Supplementary

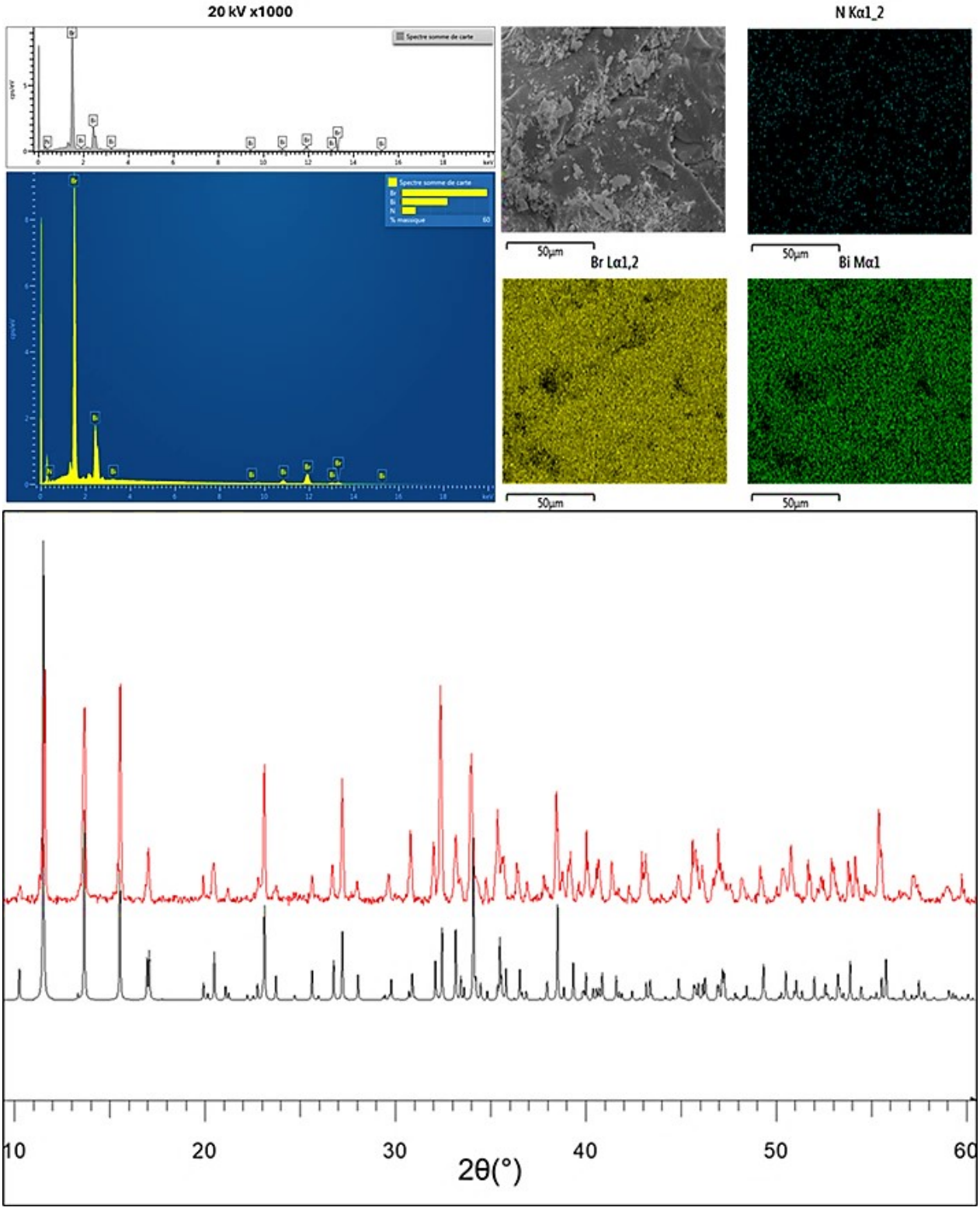

Fig. 1.S: (Upper) EDS spectrum and elemental mapping of $(C_8H_{14}N_2)_2[Bi_2Br_{10}]\cdot 2H_2O$, (Lower) PXRD pattern with experimental (red) and simulated (black) data

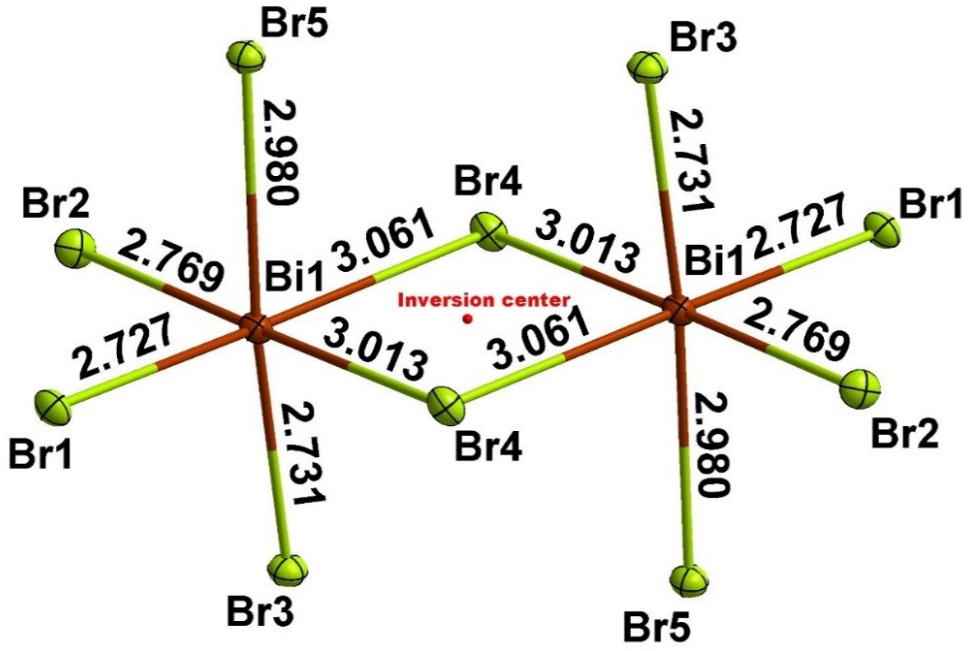

Fig. 2.S: Variations in Bi—Br Bond Lengths within the dimer

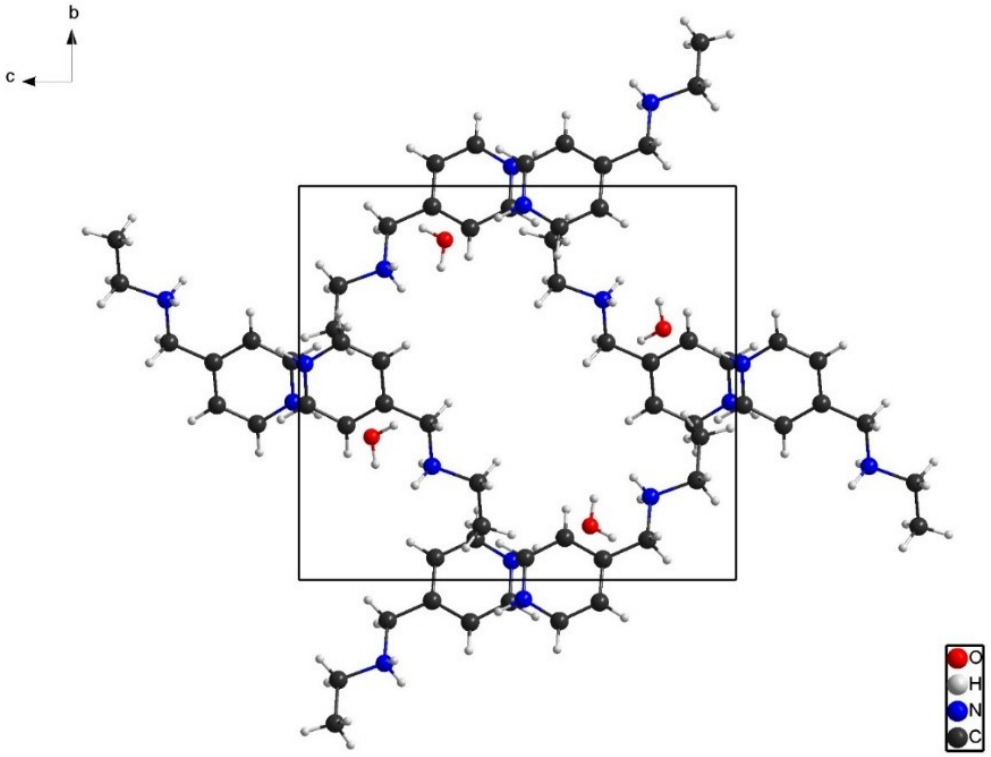

Fig. 3.S: The spatial arrangement of organic molecules within the unit cell

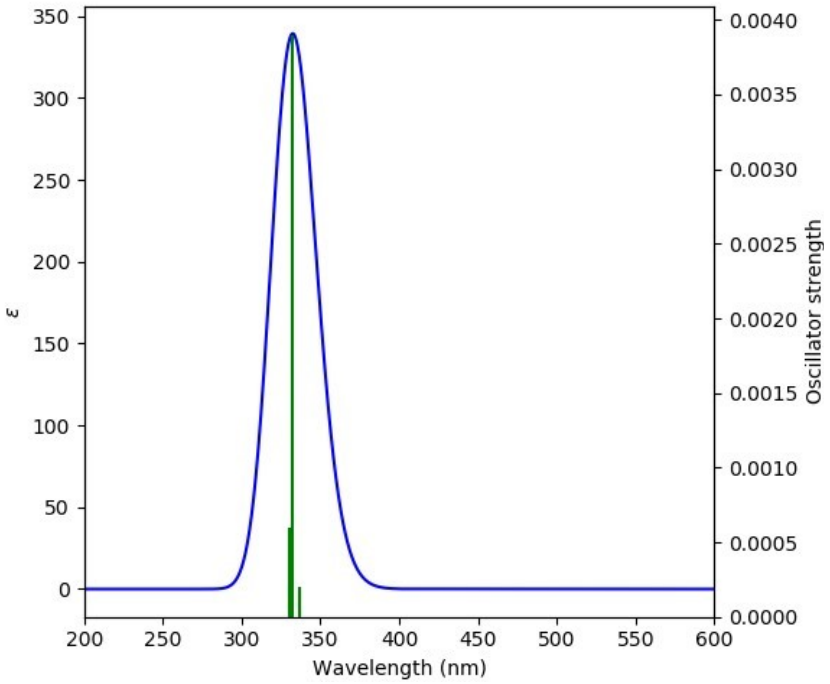

Fig. 4.S: Simulated UV-Visible spectrum

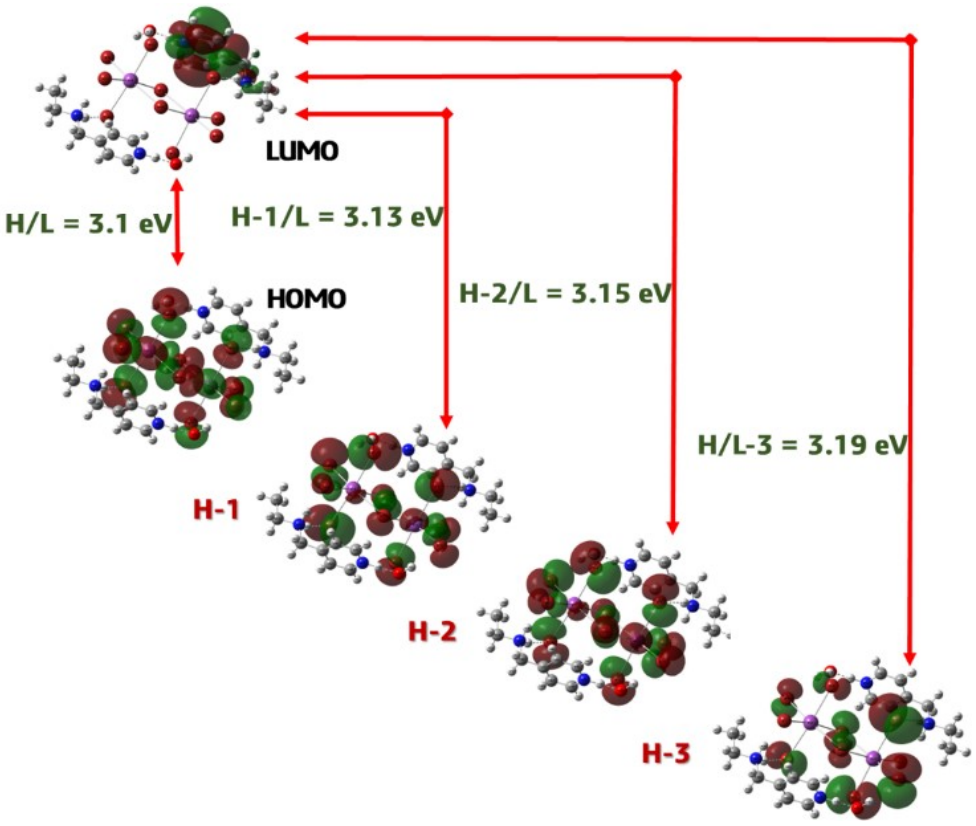

Fig. 5.S: The selected MO drawings for the compound

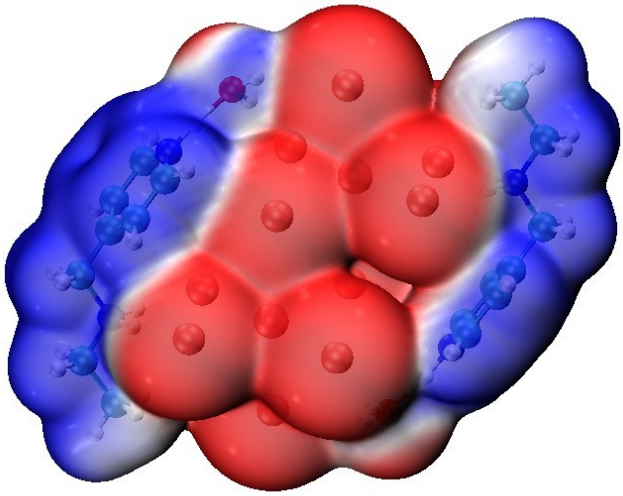

Fig. 6.S: Molecular Electrostatic Potential Analysis of the Target Compound

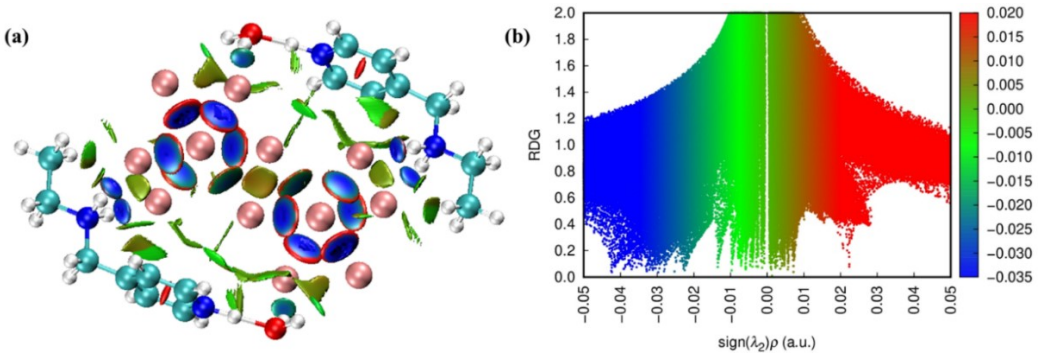

Fig. 7.S: NCI (a) and RDG (b) Visualization of the Target Compound

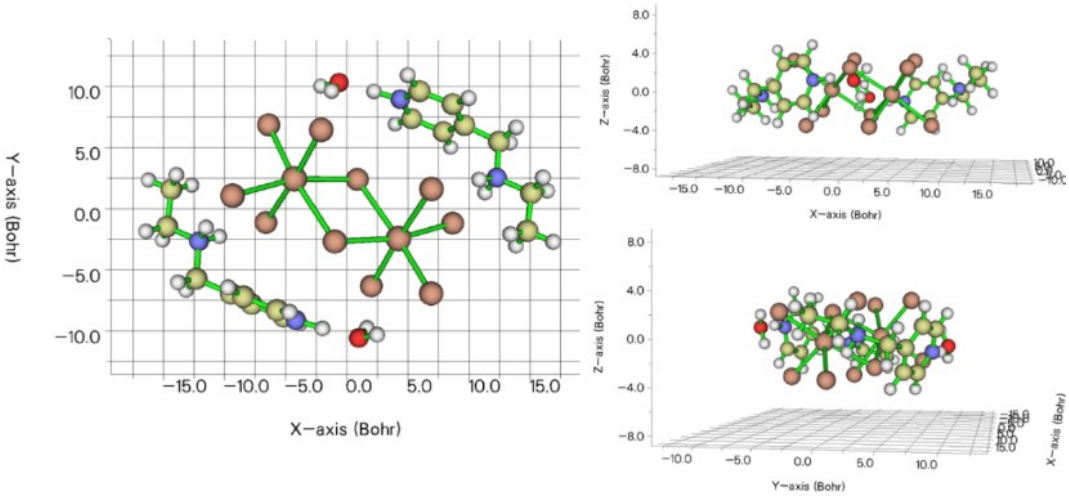

Fig. 8.S: Presentation of theoretical formula unit in (XY), (XZ), and (YZ)

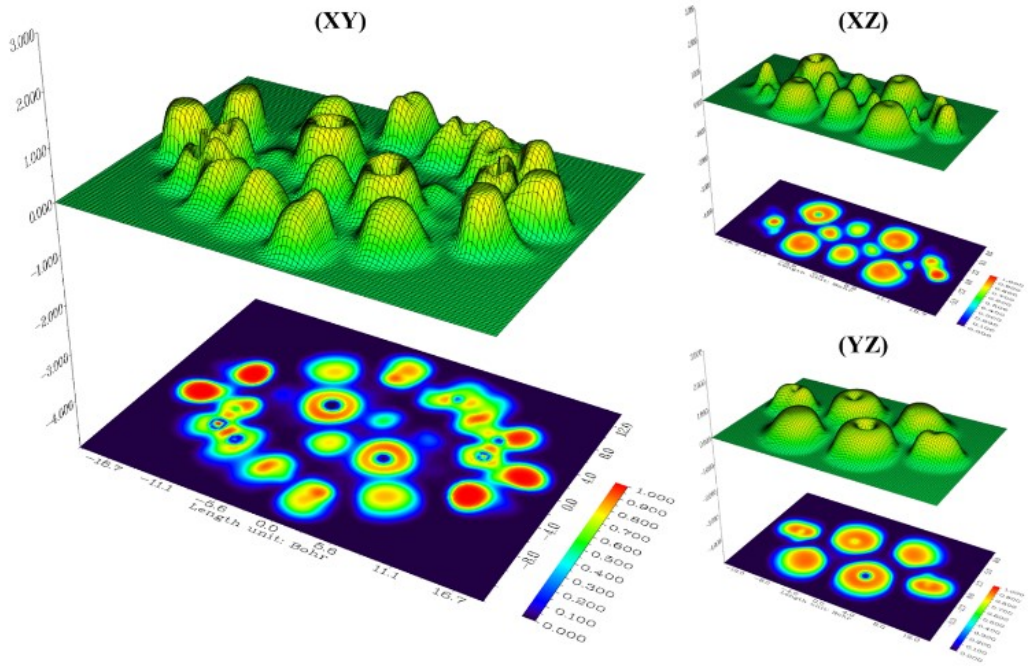

Fig. 9.S: Electron Localization Function (ELF) visualization in (XY), (XZ), and (YZ) planes

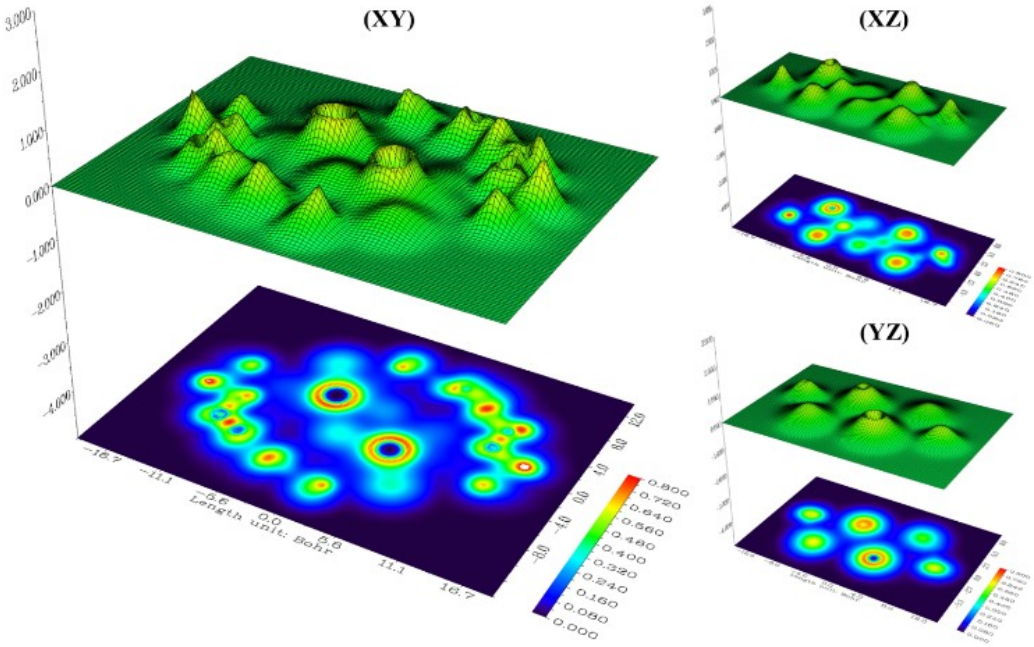

Fig. 10.S: Localized Orbital Locator (LOL) visualization in (XY), (XZ), and (YZ) planes

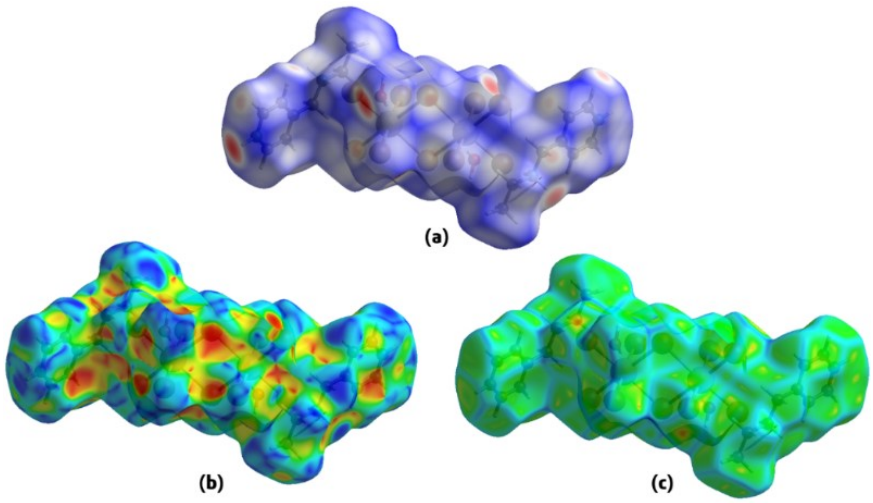

Fig. 11.S: Hirshfeld surface of the titled: **(a)** 3D dnorm surface, **(b)** surface index **(c)** curvedness

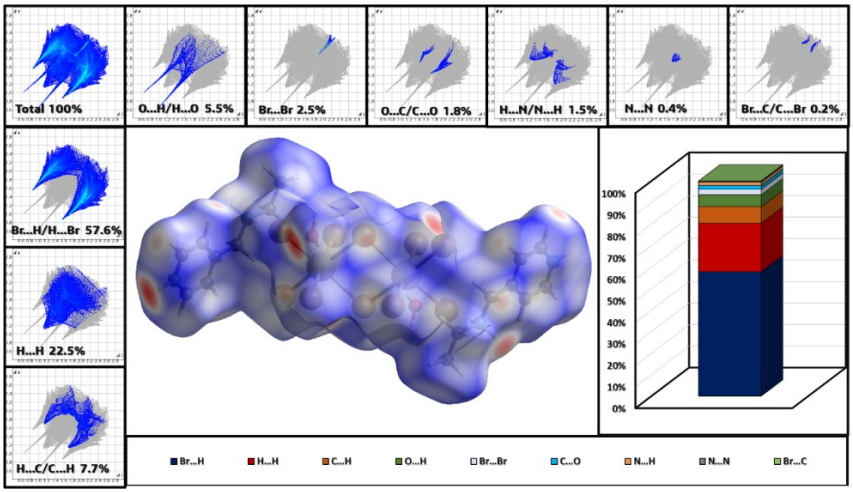

Fig. 12.S: 2D Visualization of Total Contact Contributions to the Hirshfeld Surface

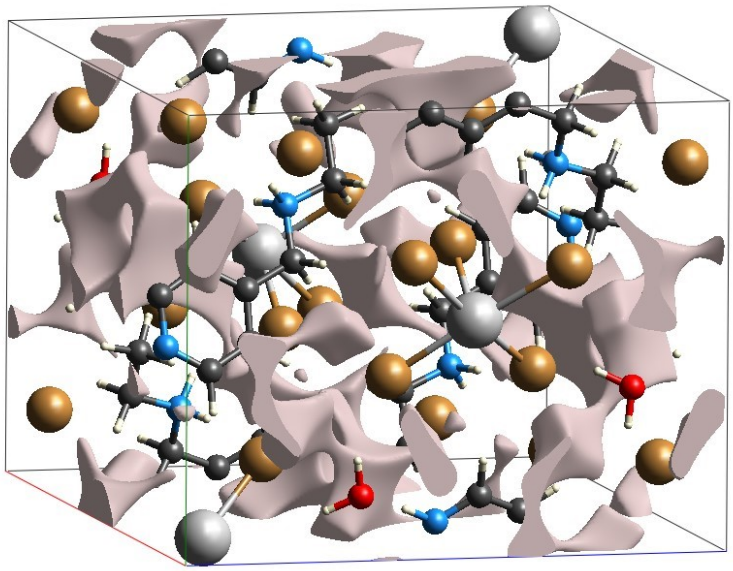

Fig. 13.S: Presence of a Crystal Void in the Compound

Table 1.S: Atomic coordinates and thermal agitation factors of the titled compound

	x	y	z	U_{iso}*/U_{eq}
Bi1	0.20051 (2)	0.48343 (2)	0.59857 (2)	0.01017 (8)
Br1	0.42518 (4)	0.60690 (4)	0.63256 (4)	0.01428 (12)
Br2	0.33532 (4)	0.34220 (4)	0.75168 (4)	0.01529 (12)
Br3	0.25221 (4)	0.35304 (4)	0.45761 (4)	0.01499 (12)
Br4	0.05793 (4)	0.64639 (4)	0.43901 (4)	0.01345 (12)
Br5	0.11876 (4)	0.61733 (4)	0.74600 (3)	0.01366 (12)
O1	0.0317 (4)	0.3629 (3)	0.8339 (3)	0.0204 (8)
H1B	0.044809	0.392330	0.783227	0.031*
H1C	0.022224	0.293388	0.824947	0.031*
N1	0.8422 (4)	0.5486 (4)	0.9866 (3)	0.0187 (9)
H1	0.874023	0.580355	1.043779	0.022*
N2	0.6263 (4)	0.2887 (3)	0.6955 (3)	0.0137 (9)
H2A	0.556955	0.295520	0.717319	0.016*
H2B	0.681940	0.239939	0.734359	0.016*
C1	0.8394 (5)	0.6042 (4)	0.9041 (4)	0.0192 (11)
H1A	0.872389	0.675997	0.909382	0.023*
C2	0.7883 (5)	0.5563 (4)	0.8122 (4)	0.0193 (11)
H2	0.785270	0.595738	0.755024	0.023*
C3	0.7406 (4)	0.4476 (4)	0.8045 (4)	0.0149 (10)
C4	0.7450 (5)	0.3928 (4)	0.8916 (4)	0.0187 (11)
H4	0.712816	0.320903	0.888529	0.022*
C5	0.7966 (5)	0.4444 (5)	0.9826 (4)	0.0204 (11)
H5	0.799943	0.407376	1.041083	0.024*
C6	0.6941 (5)	0.3976 (4)	0.7029 (4)	0.0174 (11)
H6A	0.633564	0.449109	0.658131	0.021*
H6B	0.769922	0.388799	0.679655	0.021*
C7	0.5799 (5)	0.2466 (4)	0.5899 (4)	0.0175 (11)
H7A	0.655408	0.239385	0.566045	0.021*
H7B	0.519041	0.299692	0.547562	0.021*
C8	0.5116 (5)	0.1362 (5)	0.5824 (4)	0.0226 (12)
H8A	0.475660	0.115004	0.513539	0.034*
H8B	0.441094	0.141676	0.610899	0.034*

H8C	0.574376	0.081523	0.618120	0.034*

Table 2.S: Distances and angles of chemical bonds in $[Bi_2Br_{10}]^{4-}$ anions.

Distances (Å)	
Bi1—Br1	2.7271 (5)
Bi1—Br2	2.7688 (5)
Bi1—Br3	2.7310 (5)
Bi1—Br4i	3.0612 (5)
Bi1—Br4	3.0126 (5)
Bi1—Br5	2.9800 (5)

Angles (°)	
Br1—Bi1—Br2	89.671 (15)
Br1—Bi1—Br3	94.257 (15)
Br1—Bi1—Br4	88.679 (14)
Br1—Bi1—Br4i	177.625 (14)
Br1—Bi1—Br5	90.885 (14)
Br2—Bi1—Br4	177.203 (15)
Br2—Bi1—Br4i	91.795 (14)
Br2—Bi1—Br5	88.989 (14)
Br3—Bi1—Br2	92.266 (15)
Br3—Bi1—Br4i	87.554 (14)
Br3—Bi1—Br4	90.109 (14)
Br3—Bi1—Br5	174.713 (14)
Br4—Bi1—Br4i	89.782 (13)
Br5—Bi1—Br4i	87.274 (13)
Br5—Bi1—Br4	88.778 (13)
Bi1—Br4—Bi1i	90.218 (13)

Table 3.S: Interatomic distances and chemical bond angles in $(C_8H_{14}N_2)^{2+}$ cations and H_2O molecules.

Distances (Å)	
O1—H1B	0.8504
O1—H1C	0.8505
N1—H1	0.8600
N1—C1	1.339 (7)
N1—C5	1.344 (7)
N2—H2A	0.8900
N2—H2B	0.8900
N2—C6	1.489 (6)
N2—C7	1.502 (6)
C1—H1A	0.9300
C1—C2	1.366 (8)
C2—H2	0.9300
C2—C3	1.400 (7)
C3—C4	1.385 (7)
C3—C6	1.489 (7)
C4—H4	0.9300
C4—C5	1.376 (7)
C5—H5	0.9300
C6—H6A	0.9700
C6—H6B	0.9700
C7—H7A	0.9700
C7—H7B	0.9700
C7—C8	1.507 (7)
C8—H8A	0.9600
C8—H8B	0.9600
C8—H8C	0.9600

Angles (°)	
C1—N1—H1	119.1
C1—N1—C5	121.8 (4)
C5—N1—H1	119.1
H2A—N2—H2B	108.0
C6—N2—H2A	109.3

C6—N2—H2B	109.3
C6—N2—C7	111.5 (4)
C7—N2—H2A	109.3
C7—N2—H2B	109.3
N1—C1—H1A	119.8
N1—C1—C2	120.5 (5)
C2—C1—H1A	119.8
C1—C2—H2	120.2
H1B—O1—H1C	109.4
C1—C2—C3	119.7 (5)
C3—C2—H2	120.2
C2—C3—C6	117.1 (4)
C4—C3—C2	118.1 (5)
C4—C3—C6	124.7 (5)
C3—C4—H4	119.9
C5—C4—C3	120.3 (5)
C5—C4—H4	119.9
N1—C5—C4	119.6 (5)
N1—C5—H5	120.2
C4—C5—H5	120.2
N2—C6—C3	115.5 (4)
N2—C6—H6A	108.4
N2—C6—H6B	108.4
C3—C6—H6A	108.4
C3—C6—H6B	108.4
H6A—C6—H6B	107.5
N2—C7—H7A	109.3
N2—C7—H7B	109.3
N2—C7—C8	111.5 (4)
H7A—C7—H7B	108.0
C8—C7—H7A	109.3
C8—C7—H7B	109.3
C7—C8—H8A	109.5
C7—C8—H8B	109.5

C7—C8—H8C	109.5
H8A—C8—H8B	109.5
H8A—C8—H8C	109.5
H8B—C8—H8C	109.5

Table 4.S: The attributions of calculated and observed frequencies of the vibration modes of the compound

IR (cm^{-1})	Raman (cm^{-1})	Calc. wavenumbers (cm^{-1})	Assignement
3578	**-**	**3660**	υ_{as}**(H_2O)**
3451	**-**	**3423**	υ_{s}**(H_2O)**
3345	**-**	**3386**	υ_{s}**(H_2O)**
3160	**-**	**3169**	υ_{as}**(CH_2)**
3081	**-**	**3069**	υ_{s}**(CH_3)**
3035	**-**	**2930**	υ_{as}**(NH_2)**
2814	**-**	**2841**	υ_{s}**(NH_2)**
2750	**-**	**2814**	$\upsilon(N-H)$
1845-2694	**-**	**2280-2323**	$\upsilon(N-H\ldots O)$
1720	**-**	**1772**	δ**(NH_2)**
1651	**-**	**1695**	δ**(H_2O)**
1535	**-**	**1554**	**ω(NH_2)**
1508	**-**	**1517**	**δ(CH_2)**
1415	**-**	**1448**	**τ(NH_2) +τ(CH_2)**
1342	**-**	**1344**	**ω(CH_2)**
1269	**-**	**1309**	**υ(N-C) + β_{as}(C-H)**
1213	**-**	**1249**	**β_s(C-H)**
1129	**-**	**1148**	**τ(CH_3)**
1088	**-**	**1056**	**υ_{as}(C-C-N)**
1018	**-**	**1014**	**γ_{as}(C-H)**
945	**-**	**927**	**ρ(NH_2)**
844	**-**	**853**	**γ_s(C-H)**
775	**-**	**751**	**ω(H_2O)**
585	**-**	**603**	**ρ(H_2O)**
552	**-**	**543**	**δ(C-N-C) + δ(C-C-C)**
-	**176**	**185**	υ_{as}**(Bi-Br)**
-	**154**	**160**	**ρ(Br-Bi-Br)**
-	**113**	**133**	υ_{s}**(Bi-Br)**
-	**98**	**112**	**δ(Br-Bi-Br)**
-	**74**	**78**	*lattice mode*

υ_s :$symetric\ stretching$, υ_{as} :$assymetric\ stretching$, β : $in\ plane\ bending$, γ :$out\ plane\ bending$, δ :$scissoring$, ρ :$rocking$,
ω:$wagging$, τ : Twisting

Table 4.S: Calculated global reactivity parameters of the new compound

Parameter	Value (eV)
HOMO	-6.19
LUMO	-3.09
$\mathbf{E_A}$	3.09
$\mathbf{E_I}$	6.19
μ	-4.64
η	1.55
S	2.00
ω	6.94
χ	4.64

Table 5.S: The calculated wavelengths, oscillator strengths, and major contributions for electronic transitions

Wavelength (nm)	Oscillator strength	Major contribution
336.6391	0.0002	HOMO → LUMO (88%)
332.5488	0.0039	H-2 → LUMO (76%), H-1 → LUMO (15%)
330.3162	0.0006	H-3 → LUMO (87%)