crystals

Crystal Structure and Supramolecular Architecture of Inorganic Ligand-Coordinated Salen-Type Schiff Base Complex: Insights into Halogen Bond from Theoretical Analysis and 3D Energy Framework Calculations

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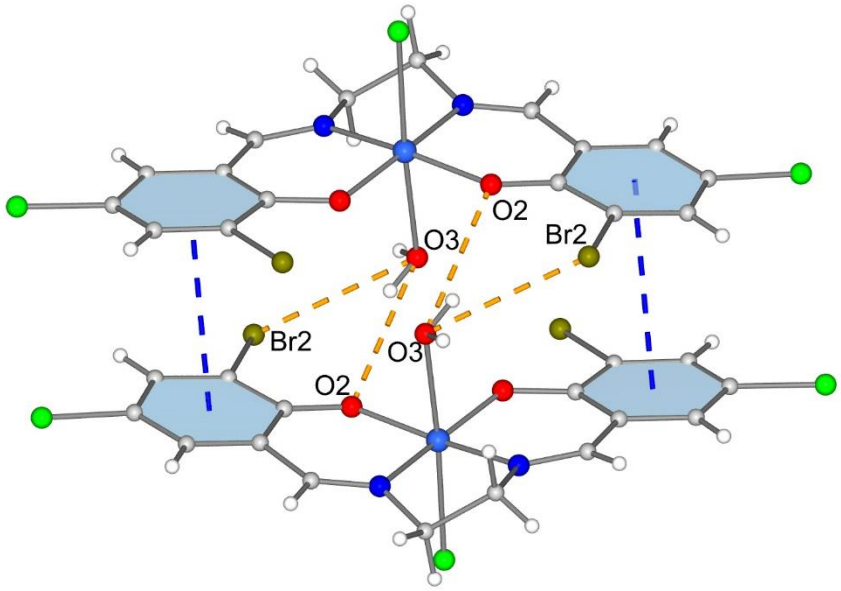

Figure S1. The self-assembled supramolecular dimer of compound **1**.

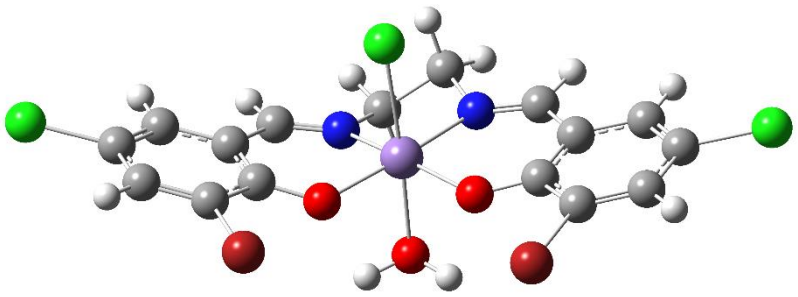

Figure S2. The optimized structure of **1**.

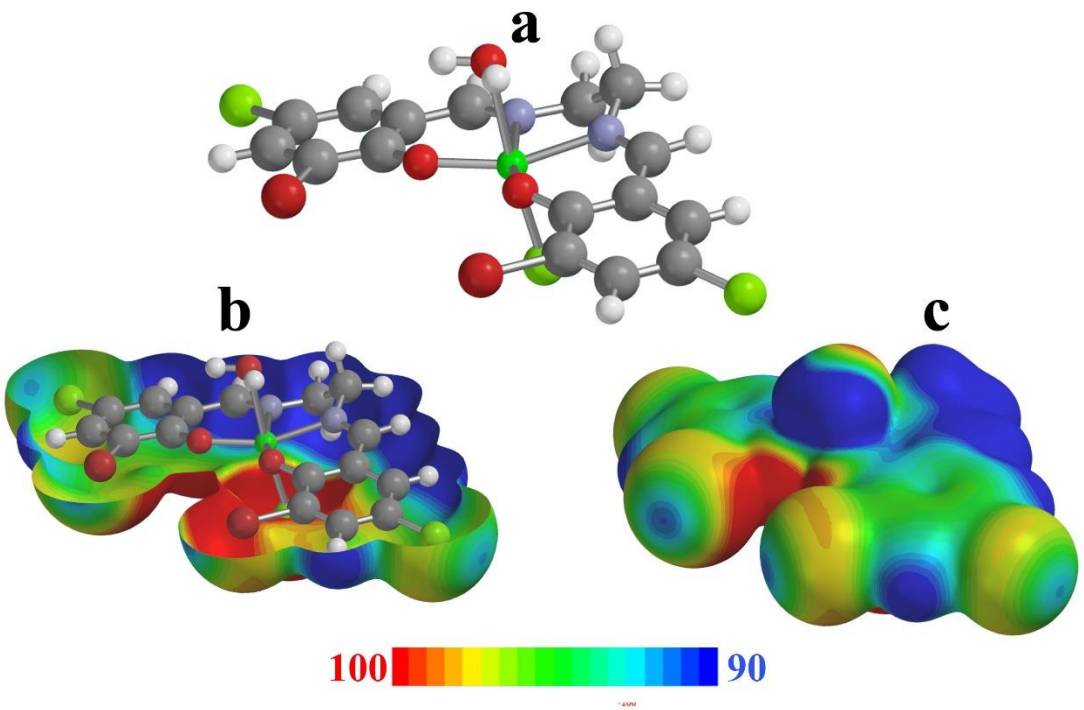

Figure S3. (**a**) The Molecular structure of **1** (**b**) full ESP in atomic units (kJ) projected onto the molecular surface (**c**). The banded property map of positive ESP in the forefront is the σ-hole.

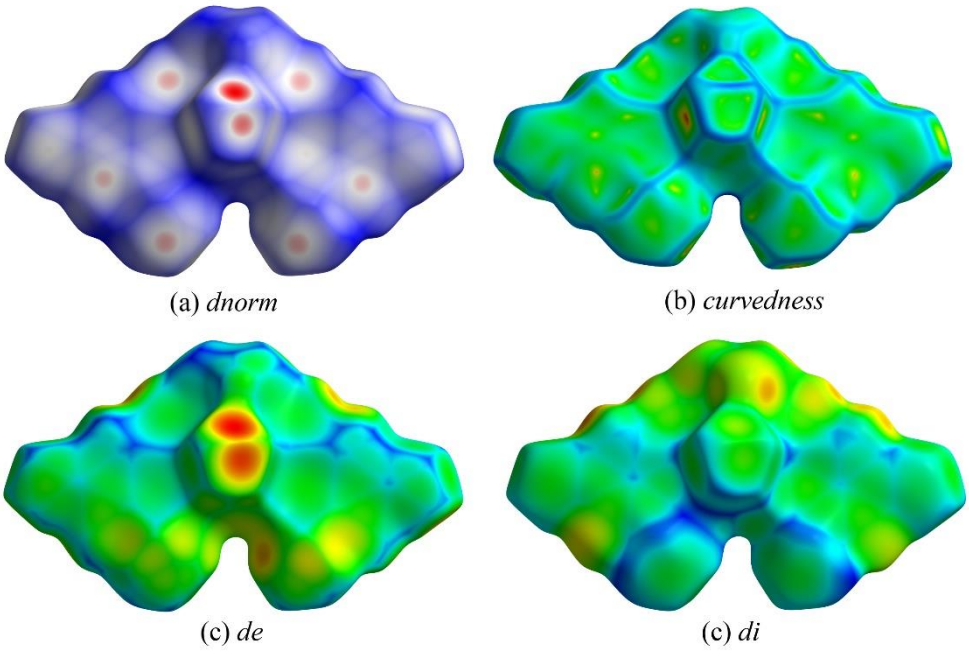

Figure S4. Hirshfeld surfaces mapped with *dnorm*, *curvedness*, *de* and *di* index of compound **1**.

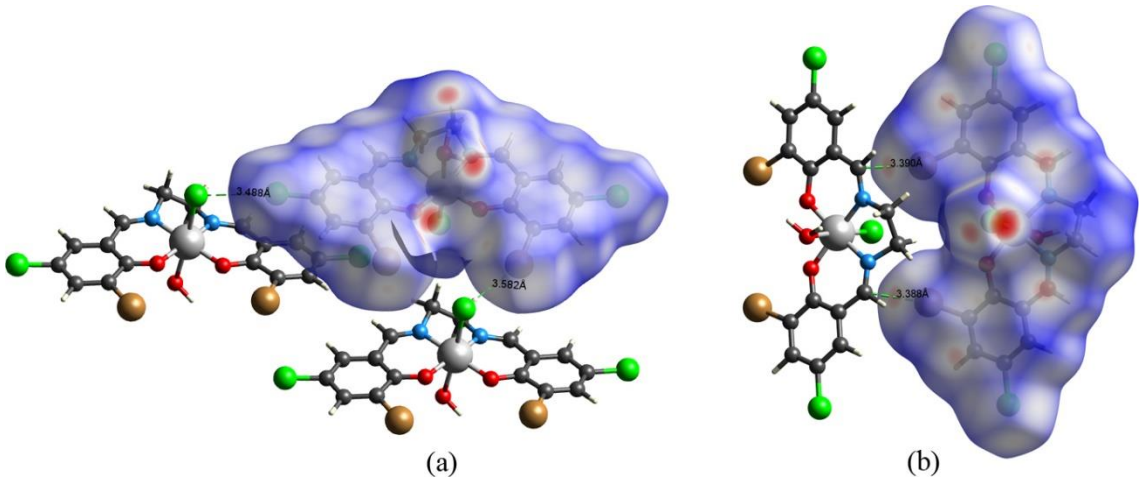

Figure S5. Shortest Cl···Cl and Cl···Br interaction in **1**. right, Shortest C···Br interaction in **1**.

Table S1. Molecular pair wise interaction energies (kJ/mol) obtained from the energy framework calculation for compound **1**.

N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep
0	x, -y+1/2, z+1/2	10.91	B3LYP/3−21G	−2.8	−4.9	−45.0	32.1
0	x, y, z	12.42	B3LYP/3−21G	1.6	−2.4	−17.9	13.7
0	x, y, z	12.42	B3LYP/3−21G	−2.1	−3.0	−18.1	16.2
0	-x, -y, -z	4.10	B3LYP/3−21G	−99.1	−35.9	−130.2	109.7
0	-x, -y, -z	12.09	B3LYP/3−21G	−16.4	−5.9	−26.0	17.0
0	-x, y+1/2, -z+1/2	8.44	B3LYP/3−21G	−60.0	−18.6	−15.3	32.8
0	x, -y+1/2, z+1/2	7.29	B3LYP/3−21G	−47.2	−16.3	−46.7	40.9
0	-x, -y, -z	12.39	B3LYP/3−21G	−18.5	−3.8	−22.7	13.0
0	-x, -y, -z	12.29	B3LYP/3−21G	20.1	−3.7	−5.0	0.1
				−224.4	−89.6	−326.9	275.5

Interaction Energies (kJ/mol).R is the distance between molecular centroids (mean atomic position) in Å.Total energies, only reported for two benchmarked energy models, are the sum of the four energy components scaled appropriately (see the scale factor table below).[B3LYP/3−21G]. Scale factors for benchmarked energy models. See Mackenzie et al. IUCrJ (2017).

Table S2. Selected X-Bond Distances and Angles.

C-X···Cl	X···Cl, Å	X···Cl-Mn, deg
C(4)-Cl(1)···Cl(3)	3.65	97.2
C(13)-Cl(2)···Cl(3)	3.49	109.1
C(2)-Br(1)···Cl(3)	3.58	98.2
C(15)-Br(2)···Cl(3)	3.87	97.1