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Electronic Supplementary Information

A tetranuclear nickel/lead complex with a salen type Schiff base: Synthesis, structure and exploration of its photosensitive Schottky barrier diode behaviour

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Table S1: Selected bond lengths (Å) of the complex.

Pb(1)-Cl(2)	2.874(5)	Pb(1)-S(1)[a]	3.373(2)
Pb(1)-O(11)	2.385(6)	Ni(1)-O(1W)	2.209(8)
Pb(1)-O(31)	2.415(6)	Ni(1)-O(11)	2.032(6)
Pb(1)-O(51)[a]	2.787(8)	Ni(1)-O(31)	2.037(6)
Pb(1)-O(131)	2.680(6)	Ni(1)-N(1)	2.041(9)
Pb(1)-O(291)	2.734(7)	Ni(1)-N(19)	2.010(7)
Pb(1)-O(51)	2.783(8)	Ni(1)-N(23)	2.020(8)
Pb(1)-N(2)	2.557(10)	Pb(1)-Ni(1)	3.469(12)

Symmetry transformations: [a] = 1-x,-y,1-z.

Table S2: Selected bond angles (°) of the complex.

Cl(2)-Pb(1)-O(11)	81.7(2)	Cl(2)-Pb(1)-S(1)[a]	94.05(12)
Cl(2)-Pb(1)-O(31)	81.9(2)	O(131)-Pb(1)-N(2)	66.1(8)
Cl(2)-Pb(1)-O(131)	73.5(2)	O(291)-Pb(1)-N(2)	76.7(8)
Cl(2)-Pb(1)-O(291)	72.5(2)	O(51)[a]-Pb(1)-O(291)	143.0(2)
O(11)-Pb(1)-O(31)	69.5(2)	O(51)-Pb(1)-N(2)	155.2(11)
O(11)-Pb(1)-O(131)	62.0(2)	O(51)[a]-Pb(1)-O(51)	66.1(3)
O(11)-Pb(1)-O(291)	126.3(2)	O(11)-Pb(1)-S(1)[a]	149.5(2)
O(11)-Pb(1)-O(51)	104.8(2)	O(131)-Pb(1)-S(1)[a]	87.76(13)
O(11)-Pb(1)-N(2)	96.6(12)	O(51)-Pb(1)-S(1)[a]	93.87(17)
O(11)-Pb(1)-O(51)[a]	79.5(2)	O(1W)-Ni(1)-O(11)	84.7(3)
O(31)-Pb(1)-O(51)	73.6(2)	O(1W)-Ni(1)-O(31)	85.6(3)
O(31)-Pb(1)-O(131)	127.8(2)	O(1W)-Ni(1)-N(1)	174.1(3)
O(31)-Pb(1)-O(291)	61.0(2)	O(1W)-Ni(1)-N(19)	90.0(3)
O(31)-Pb(1)-N(2)	103.2(8)	O(1W)-Ni(1)-N(23)	91.1(3)
O(31)-Pb(1)-O(51)[a]	119.7(2)	O(11)-Ni(1)-O(31)	84.5(2)
O(51)-Pb(1)-O(131)	135.7(3)	O(11)-Ni(1)-N(1)	89.4(3)
O(51)-Pb(1)-O(291)	80.5(2)	O(11)-Ni(1)-N(19)	90.3(3)
O(131)-Pb(1)-O(291)	142.8(2)	O(11)-Ni(1)-N(23)	172.6(3)
O(51)[a]-Pb(1)-O(131)	69.8(2)	O(31)-Ni(1)-N(1)	94.0(3)
O(51)[a]-Pb(1)-N(2)	131.4(6)	O(31)-Ni(1)-N(19)	173.4(3)
Cl(2)-Pb(1)-O(51)	150.1(2)	O(31)-Ni(1)-N(23)	89.1(3)
Cl(2)-Pb(1)-O(51)[a]	143.2(2)	N(1)-Ni(1)-N(19)	89.9(4)
N(2)-Pb(1)-S(1)[a]	72.6(13)	N(1)-Ni(1)-N(23)	94.7(5)
O(291)-Pb(1)-S(1)[a]	79.86(13)	N(19)-Ni(1)-N(23)	95.8(4)

O(51)[a]-Pb(1)-S(1)[a]	86.58(18)	O(31)-Pb(1)-S(1)[a]	140.1(2)

Symmetry transformations: [a] = 1-x,-y,1-z.

Hirshfeld surfaces

The Hirshfeld surface[1] is unique[2] for a given crystal structure provides additional insight into the intermolecular interaction of molecular crystals.[3] The 2D-fingerprint[4] plot is very important as it provides the contribution of different intermolecular interactions in crystal structure. Crystal Explorer[5] was used to determine the Hirshfeld surfaces and the associated 2D-fingerprint plots. 2D-fingerprint plots of each Hirshfeld surface were shown as plots of d_i against d_e. The normalized contact distance (d_{norm}) based on d_e and d_i was given by,

$$d_{norm} = \frac{(d_i - r_i^{vdw})}{r_i^{vdw}} + \frac{(d_e - r_e^{vdw})}{r_e^{vdw}}$$

where r_i^{vdw} and r_e^{vdw} are the van der Waals radii of the atoms. The d_{norm} values were mapped on to the Hirshfeld surface by using a red, blue and white color scheme: where red is used to highlight shorter contacts, white is used for contacts at distances around the vdW separation and blue is for longer contacts.

Hirshfeld surfaces

Hirshfeld surface of the complex, mapped over d_{norm}, shape index and curvedness, are shown in Fig. S1. Red spots on the d_{norm} surface (Fig. S1) indicate the interaction between sulphur and hydrogen atoms. Br···H, O···H and N···H contacts are also observed in the Hirshfeld surfaces as smaller visible spots of light colour. The intermolecular interactions appearing as distinct spikes in the 2D fingerprint plot are shown in Fig. S2.

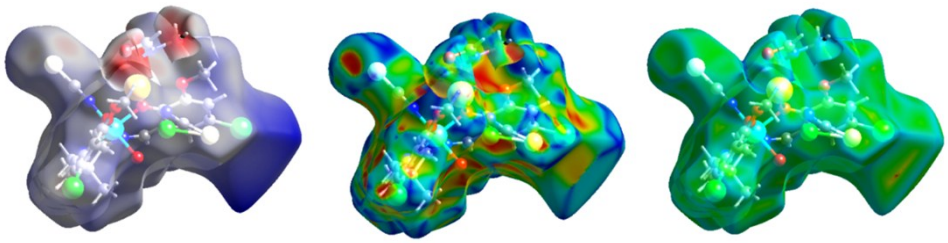

Fig. S1: Hirshfeld surfaces mapped with d_{norm} (top), shape index (middle) and curvedness (bottom) of the complex.

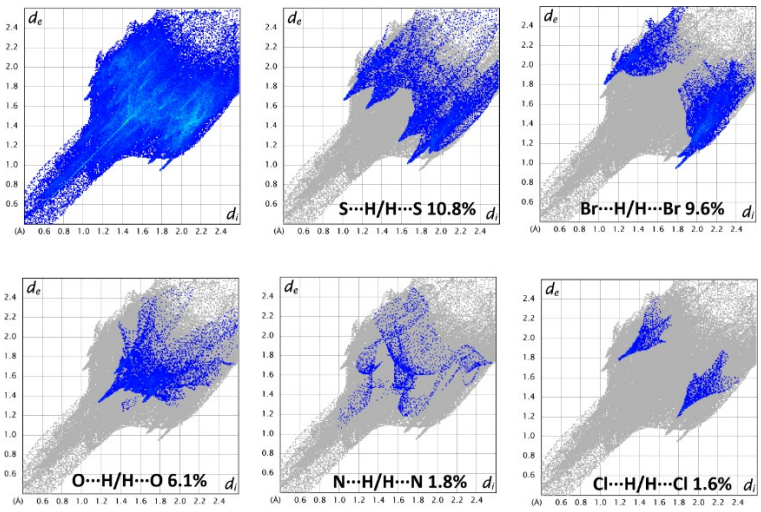

Fig. S2: Fingerprint plot: Full (top), resolved into different contacts contributed to the total Hirshfeld Surface area of the complex.

Mass Spectra

Mass spectrum (Fig. S3) of the complex has been recorded in DMF at room temperature. In the mass spectrum, peaks at m/z: 584.93, 606.91, 826.87 are observed, which may be assigned as $[Ni(L)H]^+$, $[Ni(L)Na]^+$ and $[Ni(L)Pb(Cl)]^+$ respectively.

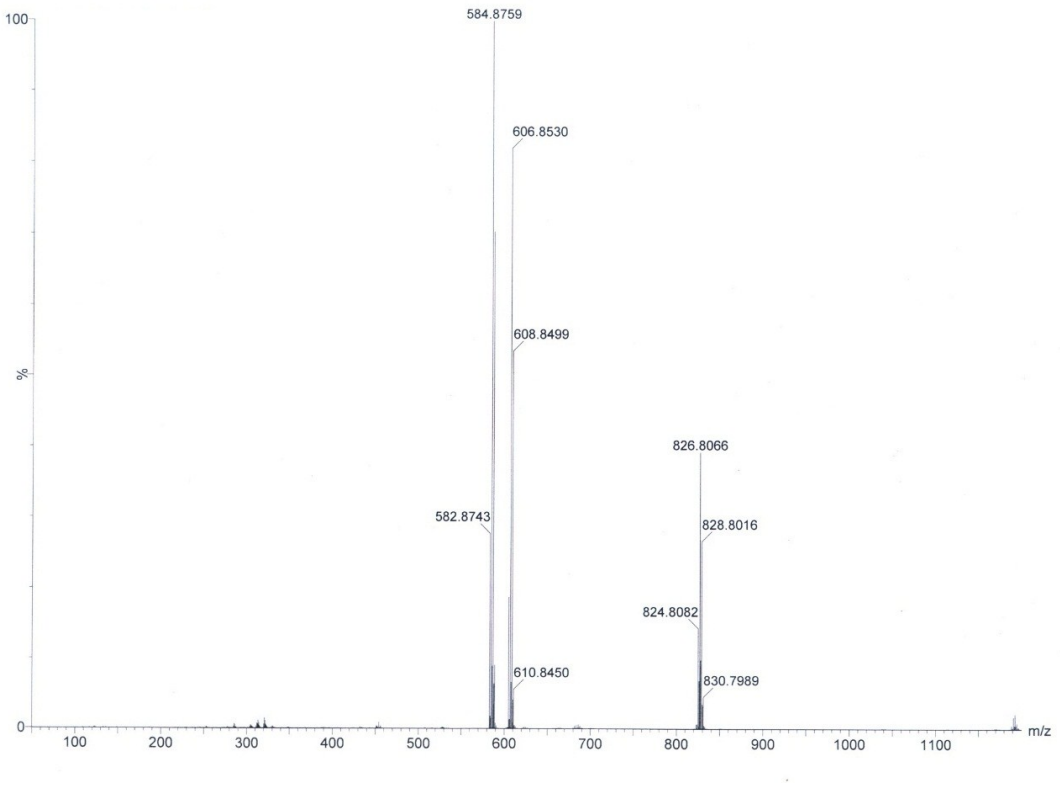

Fig. S3: Mass spectrum of the complex.

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