

# New Low-Dimensional Organic–Inorganic Lead Halide Hybrid Systems Directed by Imidazo[1,5-*a*]pyridinium-Based Cation or Imines: Synthesis, Structures, Non-Covalent Interactions and Optical Properties

Olga Yu. Vassilyeva <sup>1,\*</sup>, Elena A. Buvaylo <sup>1</sup>, Oksana V. Nesterova <sup>2</sup>, Alexandre N. Sobolev <sup>3</sup> and Dmytro S. Nesterov <sup>2,\*</sup>

<sup>1</sup> Department of Chemistry, Taras Shevchenko National University of Kyiv, 64/13 Volodymyrska Str., 01601 Kyiv, Ukraine

<sup>2</sup> Centro de Química Estrutural, Institute of Molecular Sciences, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1049-001 Lisboa, Portugal

<sup>3</sup> School of Molecular Sciences, M310, University of Western Australia, Perth, WA 6009, Australia

\* Correspondence: vassilyeva@univ.kiev.ua (O.Y.V.); dmytro.nesterov@tecnico.ulisboa.pt (D.S.N.)

## Supplementary Information

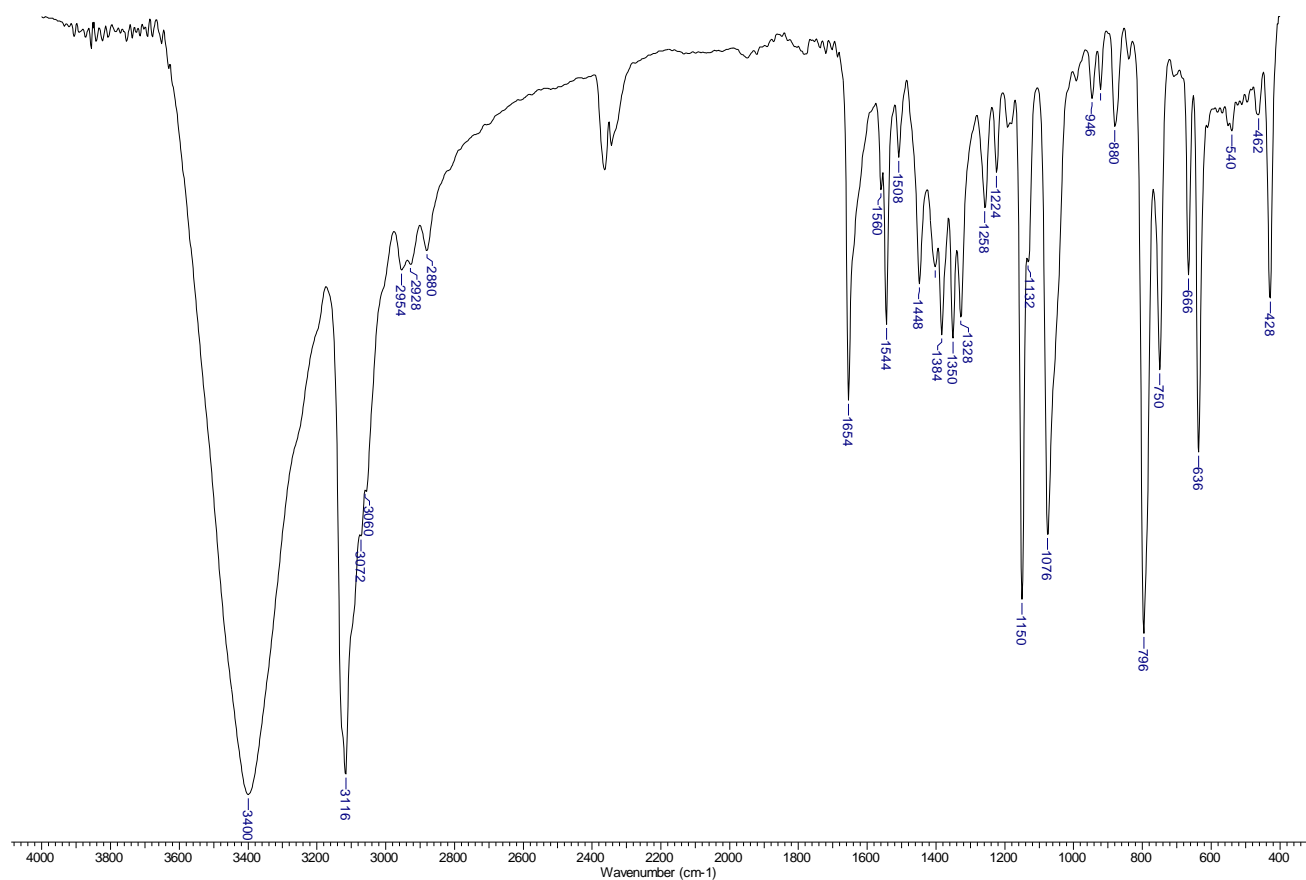


Figure S1. IR spectrum of  $[L1]_{2n}[Pb_2Cl_6]_{n\infty} \cdot nH_2O$  (**1**).

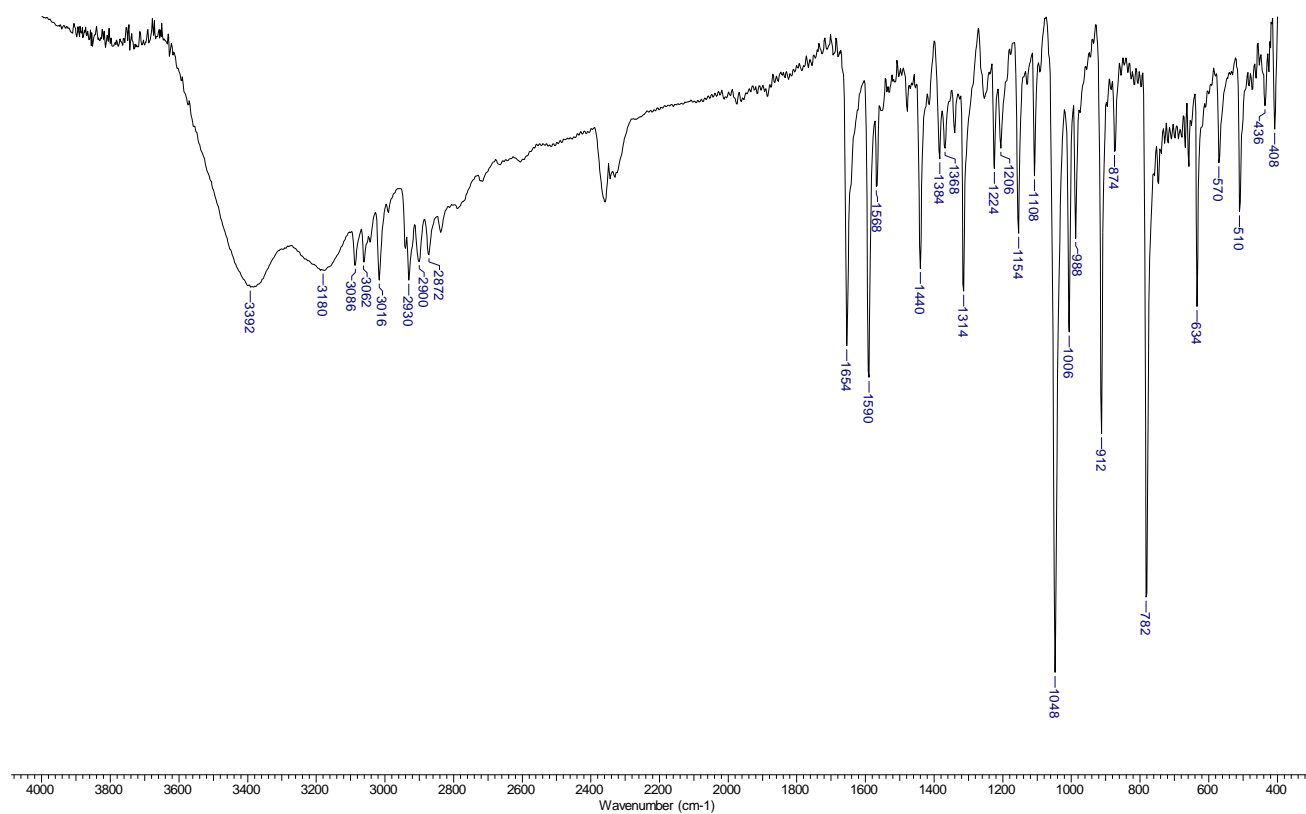


Figure S2. IR spectrum of  $[\text{PbBr}_2(\text{L2})]_n \cdot 0.5n\text{H}_2\text{O}$  (2).

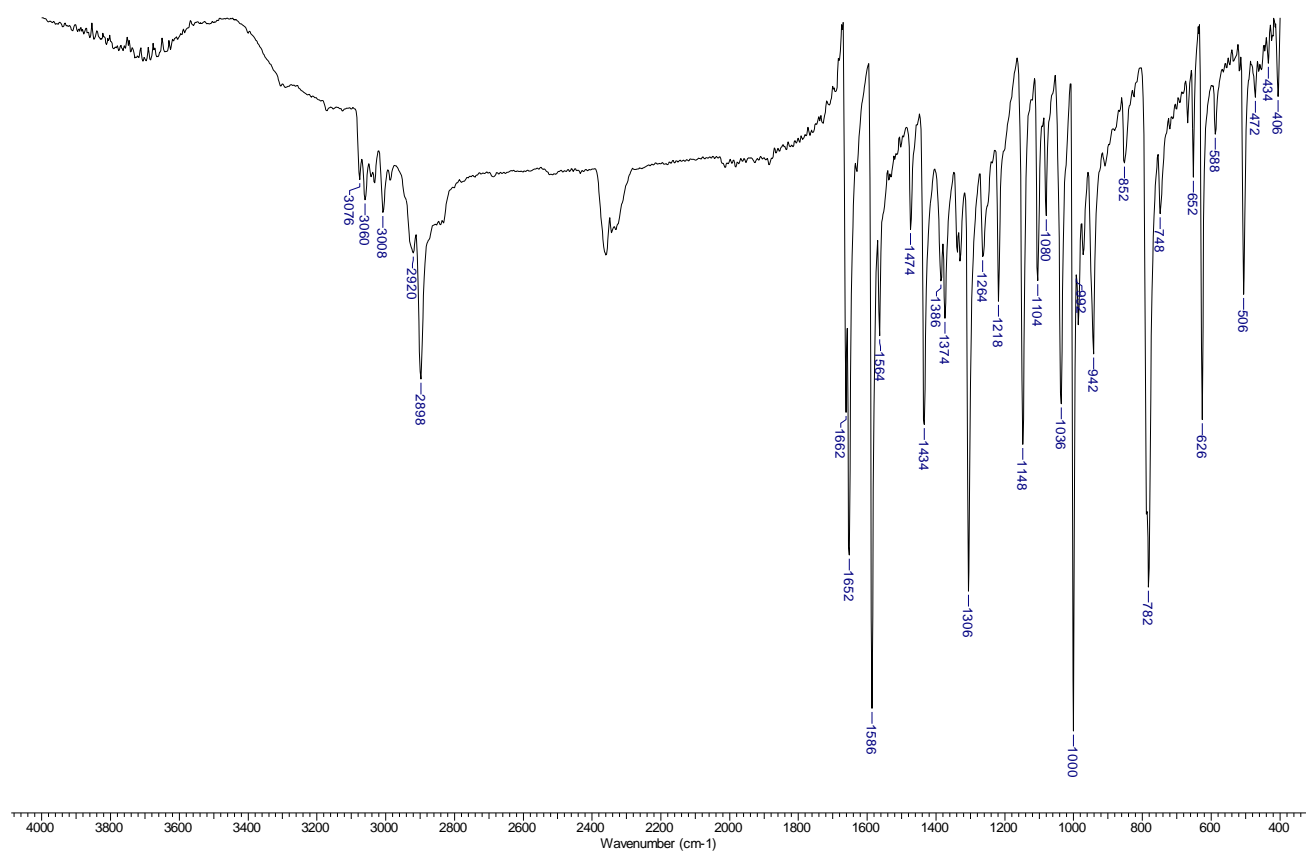


Figure S3. IR spectrum of  $[\text{PbBr}_2(\text{L3})]_2$  (3).

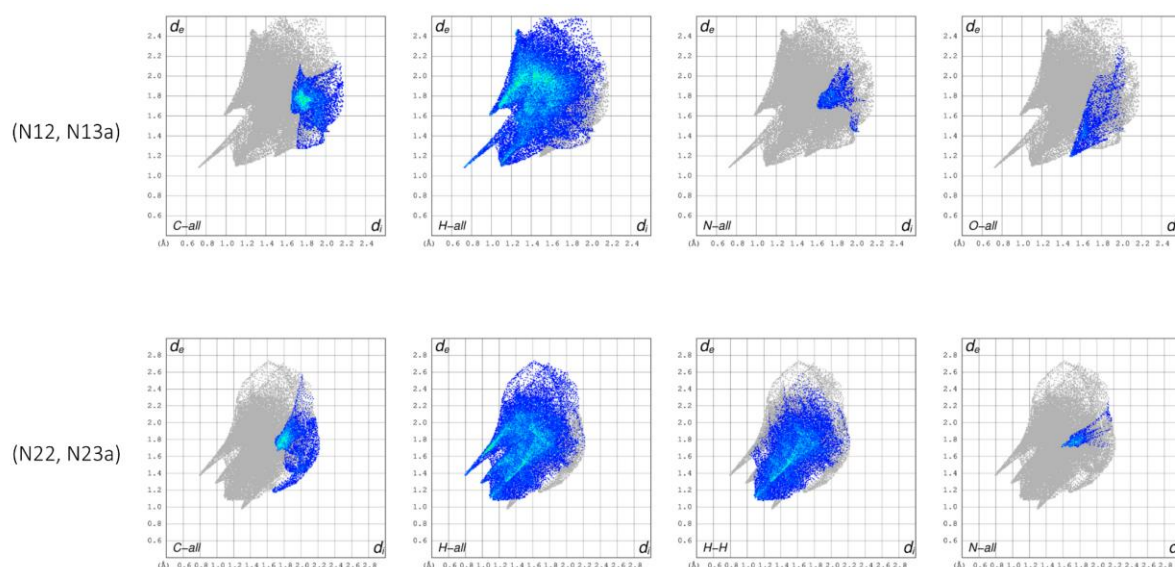


Figure S4. Selected fingerprint plots of the (N12, N13a) and (N22, N23a, major component)  $[L1]^+$  cations in the crystal structure of **1** showing  $X_i \cdots X_e$  interactions (where  $X = Cl, O, C$  or  $H$ ).

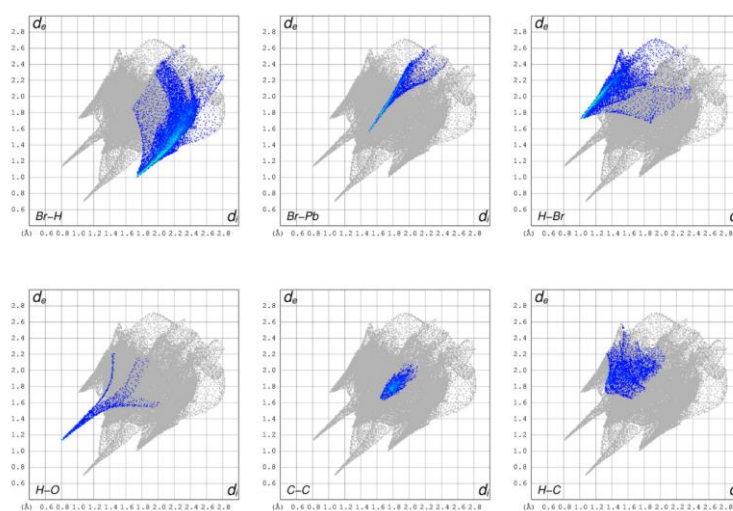


Figure S5. Selected fingerprint plots of the fragment  $[PbBr_2(L2)]$  in the crystal structure of **2** showing  $X_i \cdots X_e$  interactions (where  $X = Br, O, C$  or  $H$ ).

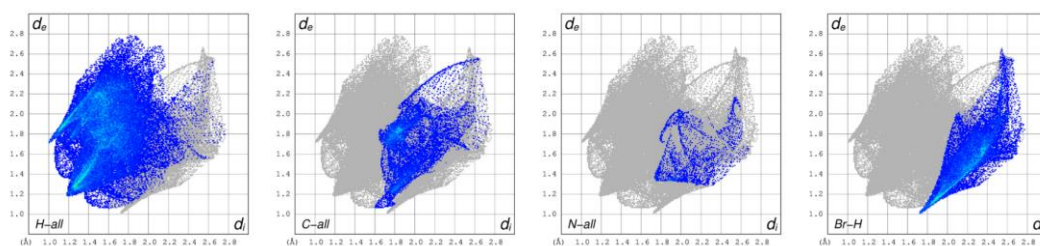


Figure S6. Selected fingerprint plots of the dinuclear molecule of **3** showing  $X_i \cdots X_e$  interactions (where  $X = Br, N, C$  or  $H$ ).

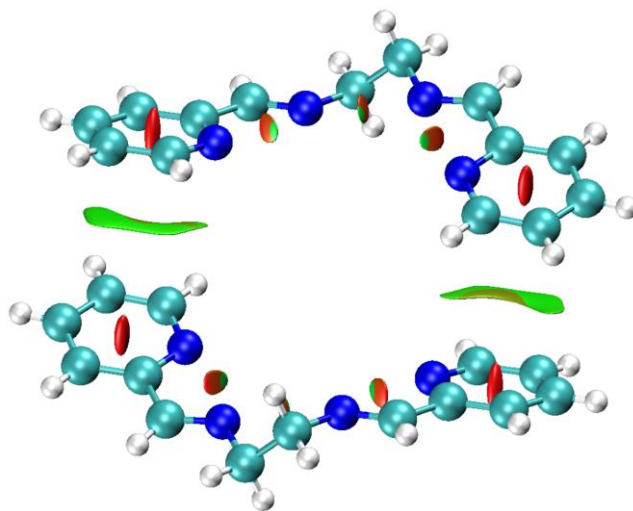


Figure S7. Reduced density gradient surfaces (isovalue of 0.5) showing weak vdW interactions (green area) between aromatic fragments of the ligands L3 in the molecular structure of **3** (lead and bromine atoms were excluded from calculations).