

## Supplementary Information File for manuscript:

### **From Monomers to Polymers: Steric and Supramolecular Effects on Dimensionality of Coordination Architectures in Heteroleptic Mercury(II) Halogenide – Tetradentate Schiff Base Complexes**

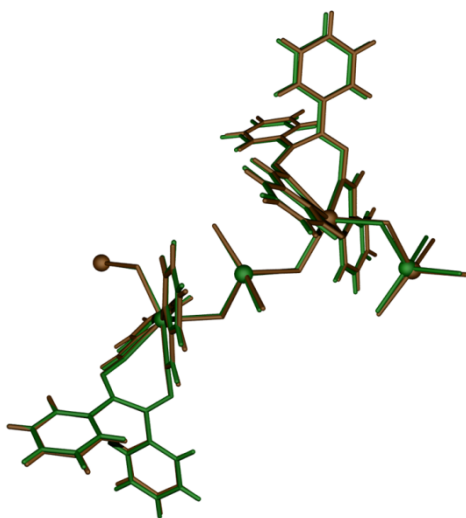
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## 1. Figure S1:

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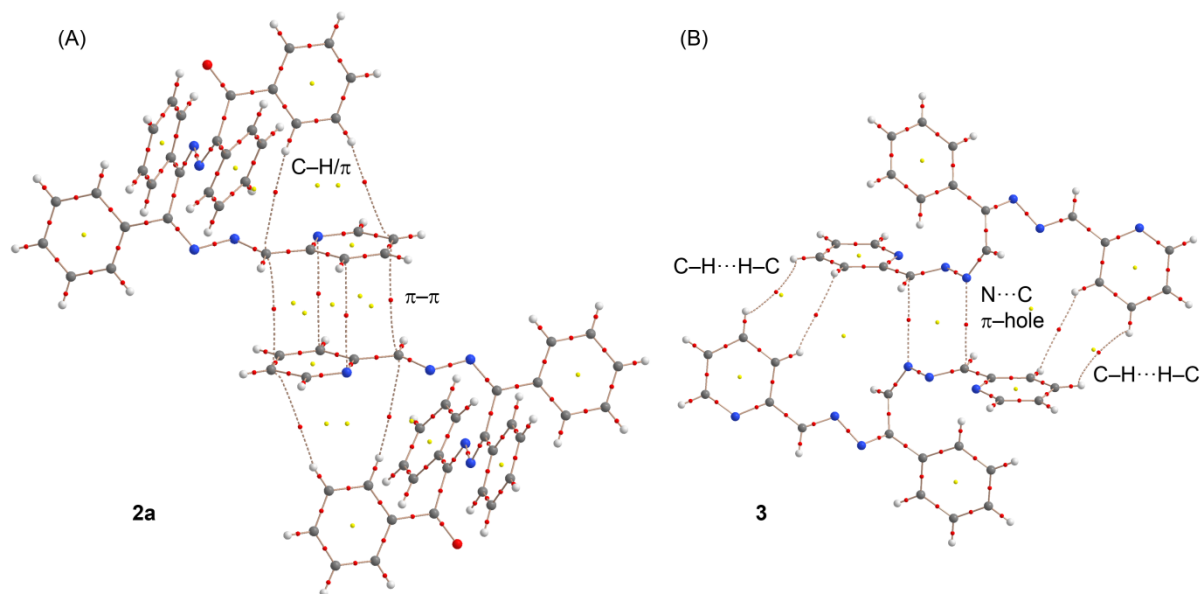


**Fig. S1** Overlap of chain sections of **2** (brown) and the chloride analogue (green). Mercury atoms are shown as small spheres.

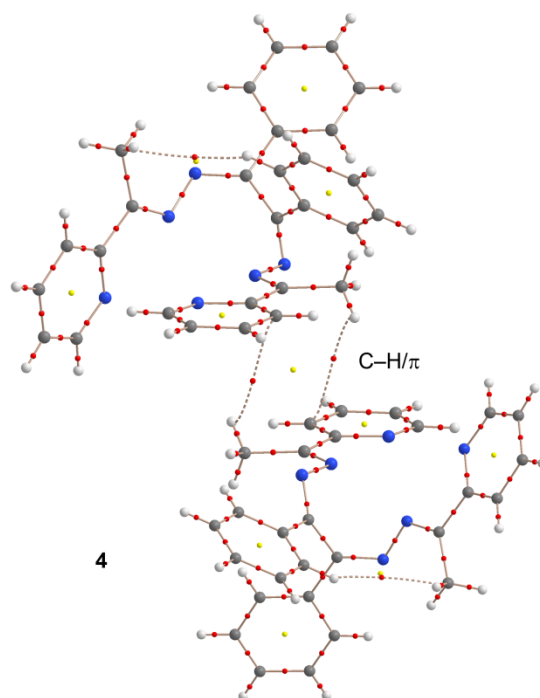
## 2. AIM analysis

The C–H $\cdots$  $\pi$ / $\pi$  $\cdots$  $\pi$ / $\pi$  $\cdots$ H–C supramolecular assembly observed in complex **2a** is characterized by several bond and ring critical points (see Fig. S2A). The intramolecular C–H $\cdots$  $\pi$  interaction is characterized by the presence of two bond critical points that connect two aromatic hydrogen atoms of the phenyl ring with two carbon atoms of the imino-pyridine extended  $\pi$ -system. Moreover the intermolecular  $\pi$ – $\pi$  interaction is characterized by the presence of four critical points that connect three carbon atoms and one nitrogen atom belonging to the imino-pyridine moiety of one ligand to the symmetrically related atoms of the other ligand. In complex **3** the double  $\pi$ -hole interaction is characterized by the presence of two symmetric bond critical points connecting the N and C atoms. The interaction is further characterized by the presence of a ring critical point that is generated as a consequence of the formation of a supramolecular six membered ring. The AIM analysis of compound **3** also reveals the existence of C–H $\cdots$ H–C interactions between the pyridine rings which also contribute to the stabilization of the dimer.

The AIM analysis of compound **4** is shown in Fig. S2. The self-complementary CH<sub>3</sub> $\cdots$  $\pi$  interaction is characterized by the presence of a bond critical point that connects one hydrogen atom of the methyl group with one carbon of the aromatic ring. For all dimers studied, the Laplacian of the electron density computed at the bond critical points is positive, as is common in closed shell interactions.<sup>42</sup>



**Fig. S2** Distribution of bond and ring critical points (red and yellow spheres, respectively) and bond paths connecting the bond critical points is represented for the supramolecular dimers observed in the solid state of compounds **2a** and **3**.



**Fig. S3** The distribution of bond and ring critical points (red and yellow spheres, respectively) and bond paths connecting the bond critical points is represented for the supramolecular dimer observed in the solid state of compound **4**.