Poster Presentation

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How C–H-based interactions affect the packing of mercury halide complexes

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In the presence study, the organic ligand (2-naphtyl pyridine-2-carboxylate) (L), which was designed to make exclusive C–H based interactions, was employed for the synthesis of three new mercury (II) halide complexes, [Hg(L)2Cl2] (1), [Hg(L)Br2] (2) and [Hg(L)I2] (3). All of the compounds were fully characterized using FT-IR, TGA, DSC, mass spectrometry, CHNS elemental analyses, PXRD, NMR and SCXRD. Interestingly, the crystal structure analysis revealed that the coordination geometry of metal center and structural motifs of complexes have been affected by accompanying anions. Furthermore, the repetitivity of C-H based interactions (e.g. C-H•••O and C–H•••π) in coordination compounds emphasized to the critical role of these weak interactions in the stability of self-assembly process. The coordination geometry around the Hg (II) ion has seesaw shape in distorted tetrahedral geometry for (1) with a τ4 index of 0.727, while there is geometry of square-based pyramid for (2) and (3) with a trigonality index, τ5 of 0.037 and 0.082 respectively. In the case of (2) and (3) the 1D linear chain are constructed as a consequence of one dimensional coordination polymers. The resulting 1D chain is linked together by the weak C–H based interactions between adjacent organic ligands to generate two distinct inorganic-organic zones in the crystal packing. In the structure of (1) the coordination environment of Hg atom consists of two crystallography independent ligands and two chloride ions. The discrete molecules of (1) are also engaged in the similar weak interactions to represent a unique combination of weak forces that contributes to the self-assembly process. The titled structures clearly illustrate how weak C–H based interactions play an important role in the 2D and 3D packing of metal complexes by the formation of repeatability supramolecular associations.

[1] Desiraju. G. R. et al. (2011) Crystal Engineering: A Textbook, World Scientific, Singapore.
[2] Khavasi. H. R. et al. (2011) CrystEngComm. 13, 3710-3717.
[3] Rahmani, M. et al. (2016) CrystEngComm, 18, 8953-8960.

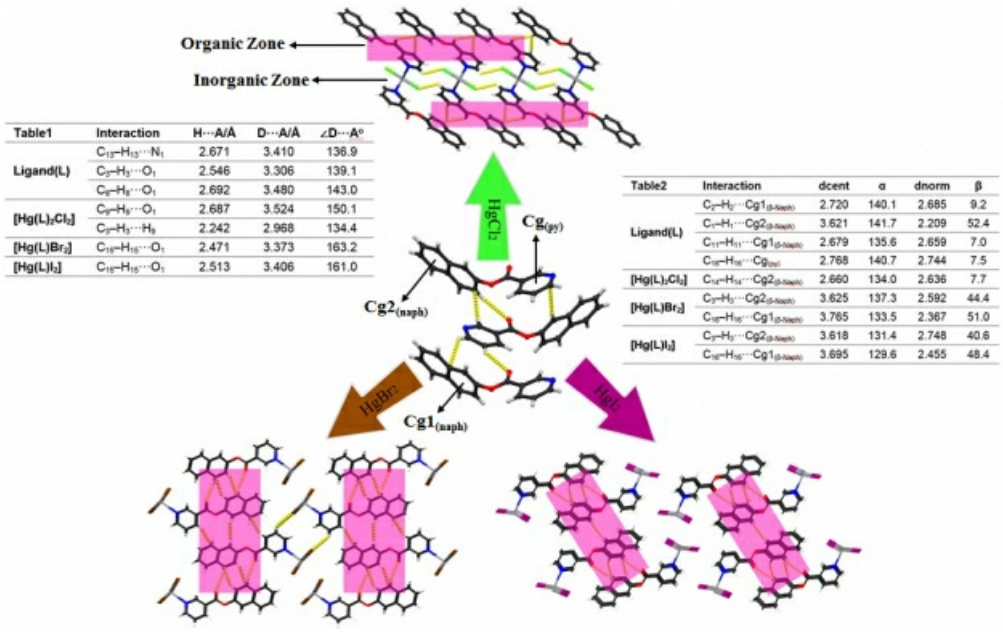

Table1	Interaction	H···A/Å	D···A/Å	∠D···A°
Ligand(L)	C_{13}–H_{13}···N_1	2.671	3.410	136.9
	C_2–H_2···O_1	2.546	3.306	139.1
	C_6–H_6···O_1	2.692	3.480	143.0
[Hg(L)$_2$Cl$_2$]	C_9–H_9···O_1	2.687	3.524	150.1
	C_5–H_5···H_9	2.242	2.968	134.4
[Hg(L)Br$_2$]	C_{15}–H_{15}···O_1	2.471	3.373	163.2
[Hg(L)I$_2$]	C_{15}–H_{15}···O_1	2.513	3.406	161.0

Table2	Interaction	dcent	α	dnorm	β
Ligand(L)	C_2–H_2···$Cg1_{(β-Naph)}$	2.720	140.1	2.685	9.2
	C_{11}–H_{11}···$Cg2_{(β-Naph)}$	3.621	141.7	2.209	52.4
	C_{11}–H_{11}···$Cg1_{(β-Naph)}$	2.679	135.6	2.659	7.0
	C_{16}–H_{16}···$Cg_{(py)}$	2.768	140.7	2.744	7.5
[Hg(L)$_2$Cl$_2$]	C_{14}–H_{14}···$Cg2_{(β-Naph)}$	2.660	134.0	2.636	7.7
[Hg(L)Br$_2$]	C_2–H_2···$Cg2_{(β-Naph)}$	3.625	137.3	2.592	44.4
	C_{16}–H_{16}···$Cg1_{(β-Naph)}$	3.765	133.5	2.367	51.0
[Hg(L)I$_2$]	C_2–H_2···$Cg2_{(β-Naph)}$	3.618	131.4	2.748	40.6
	C_{16}–H_{16}···$Cg1_{(β-Naph)}$	3.695	129.6	2.455	48.4

Keywords: crystal engineering, weak intermolecular interaction, metal complexes