

Supplementary Materials

The solvent effect on composition and dimensionality of mercury(II) complexes with picolinic acid

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1. Crystal structures

Table S1. Selected bond lengths (Å) and angles (°) for {[HgCl(pic)]}_n (**1**), [HgCl(pic)(picH)] (**2**) and [HgBr(pic)(picH)] (**3**).

1		2		3	
<i>Bond lengths</i>					
Hg1–Cl1	2.335(2)	Hg1–Cl1	2.352(2)	Hg1–Br1	2.461(2)
Hg1–N1	2.191(5)	Hg1–N1	2.212(5)	Hg1–N1	2.23(1)
Hg1–O1	2.411(4)	Hg1–N2	2.346(6)	Hg1–N2	2.33(1)
Hg1–O2 ⁱ	2.373(4)	Hg1–O1	2.487(4)	Hg1–O1	2.47(1)
		Hg1–O3	2.539(4)	Hg1–O3	2.52(1)
<i>Bond angles</i>					
N1–Hg1–Cl1	147.0(1)	N1–Hg1–N2	115.3(2)	N1–Hg1–N2	114.2(4)
N1–Hg1–O2 ⁱ	96.7(2)	N1–Hg1–Cl1	140.6(1)	N1–Hg1–Br1	137.7(3)
Cl1–Hg1–O2 ⁱ	114.8(1)	N2–Hg1–Cl1	104.1(1)	N2–Hg1–Br1	108.1(3)
N1–Hg1–O1	72.6(2)	N1–Hg1–O1	71.7(2)	N1–Hg1–O1	71.6(4)
Cl1–Hg1–O1	119.0(1)	N2–Hg1–O1	88.6(2)	N2–Hg1–O1	87.9(4)
O2 ⁱ –Hg1–O1	82.7(1)	Cl1–Hg1–O1	112.1(1)	Br1–Hg1–O1	111.5(3)
		N1–Hg1–O3	84.3(2)	N1–Hg1–O3	85.1(3)
		N2–Hg1–O3	68.4(2)	N2–Hg1–O3	68.7(4)
		Cl1–Hg1–O3	110.1(1)	Br1–Hg1–O3	110.3(3)
		O1–Hg1–O3	135.7(2)	O1–Hg1–O3	136.7(3)

Symmetry code (i) $x, -y+3/2, z+1/2$.

Table S2. The hydrogen bond geometry for {[HgCl(pic)]}_n (**1**), [HgCl(pic)(picH)] (**2**) and [HgBr(pic)(picH)] (**3**).

	D–H...A	$d(\text{D–H})/\text{\AA}$	$d(\text{H...A})/\text{\AA}$	$d(\text{D...A})/\text{\AA}$	$\angle(\text{D–H...A})^\circ$	Symmetry code on A
2						
	O4–H41...O2	0.84(1)	1.61(1)	2.451(6)	175(8)	$x+1, y, z$
3						
	O4–H41...O2	0.84	1.61	2.43(1)	163	$x-1, y, z$

2. IR spectroscopy

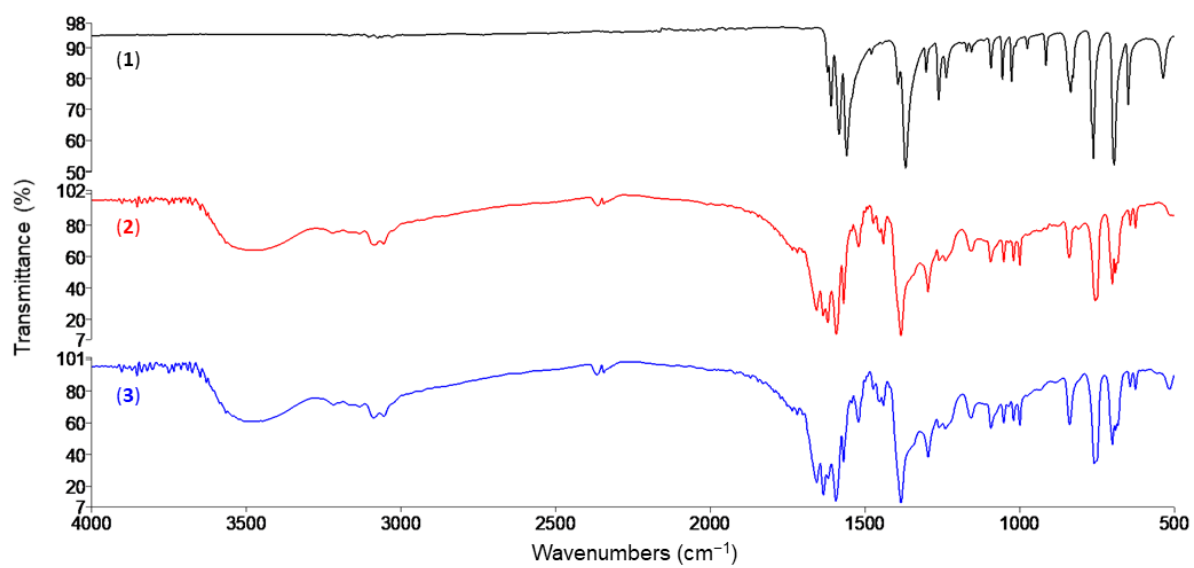


Figure S1. IR spectra of $\{[\text{HgCl}(\text{pic})]\}_n$ (**1**), $[\text{HgCl}(\text{pic})(\text{picH})]$ (**2**) and $[\text{HgBr}(\text{pic})(\text{picH})]$ (**3**).

3. TG/DSC analysis

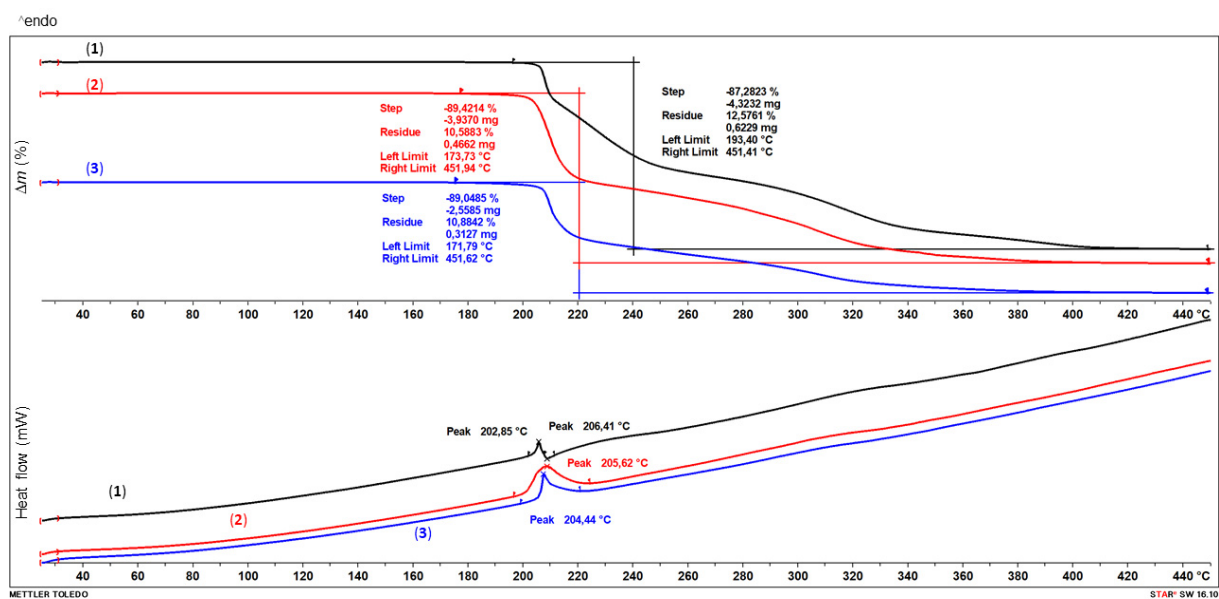


Figure S2. TGA/DSC curves of $\{[\text{HgCl}(\text{pic})]\}_n$ (1), $[\text{HgCl}(\text{pic})(\text{picH})]$ (2) and $[\text{HgBr}(\text{pic})(\text{picH})]$ (3).