Coordination complexes of *N*-((4-pyridyl)methyl)-1,8-naphthalimide and divalent metal halides: Structures and Solid State Fluorescence

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Supplementary Information

Section 1: Comparison of calculated and experimental powder X-ray diffraction patterns

Experimental powder X-ray patterns of the bulk samples were compared with powder patterns calculated from the single crystal structures determined in the study, or from the structures reported in the Cambridge Structural Database [1], in order to determine if the single crystal is representative of the bulk sample. The experimental powder patterns of **4-pn** and the **4-pnMX** complexes are shown below and compared to the corresponding calculated patterns. The experimental powder patterns are shown in black and the calculated patterns are given in red. Due to fluorescence, an increase in background intensity may occur in the experimental powder X-ray diffraction patterns of Co(II)-containing compounds at low 2θ angles.

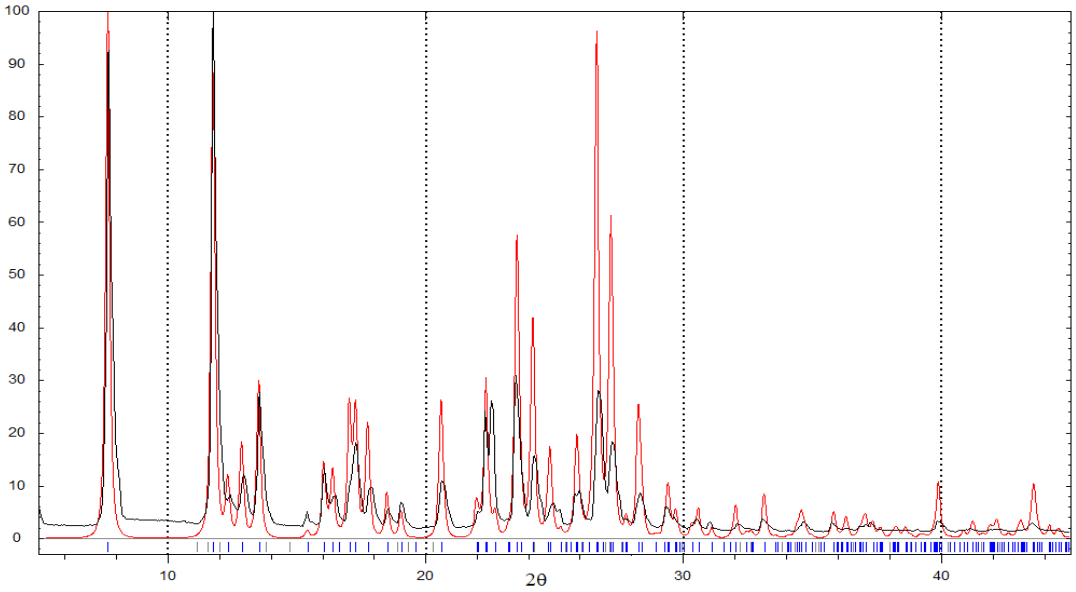

Fig. S1.1 Experimental powder pattern of *N*-((4-pyridyl)methyl)-1,8-naphthalimide, **4-pn**, compared with powder pattern calculated from the single crystal structure WEZDAH [2] reported in literature.

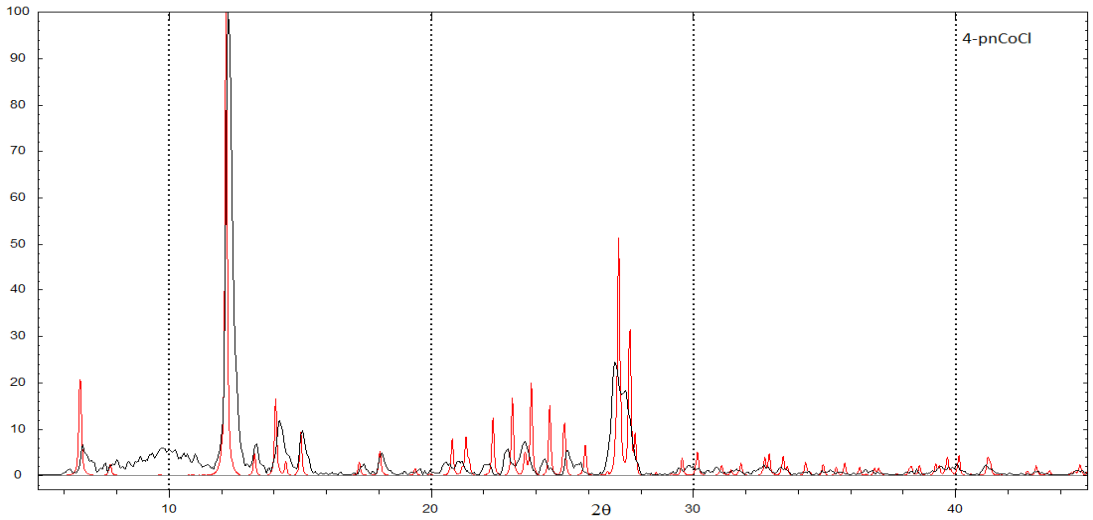

Fig. S1.2 Experimental powder pattern of **4-pnCoCl** compared with the powder pattern calculated from the single crystal structure. Intensity due to fluorescence is visible in the low angle region.

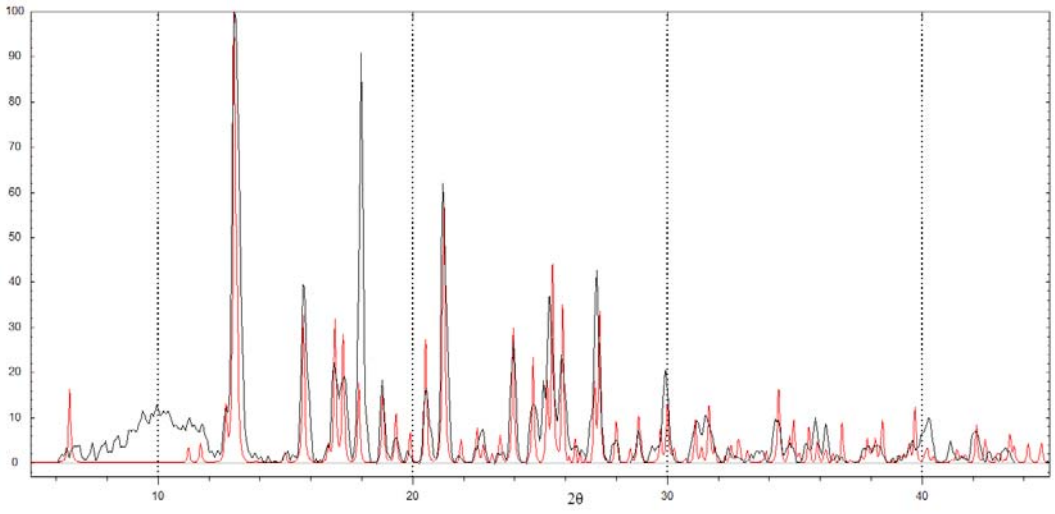

Fig. S1.3 Experimental powder pattern of **4-pnCoBr** compared with the powder pattern calculated from the single crystal structure. Intensity due to fluorescence is visible in the low angle region.

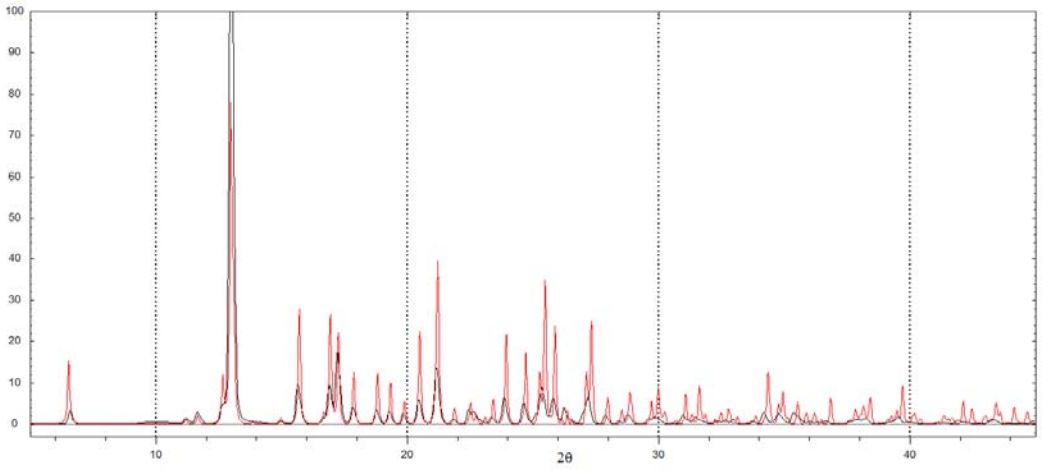

Fig. S1.4 Experimental powder pattern of **4-pnZnBr** compared with the powder pattern calculated from the single crystal structure.

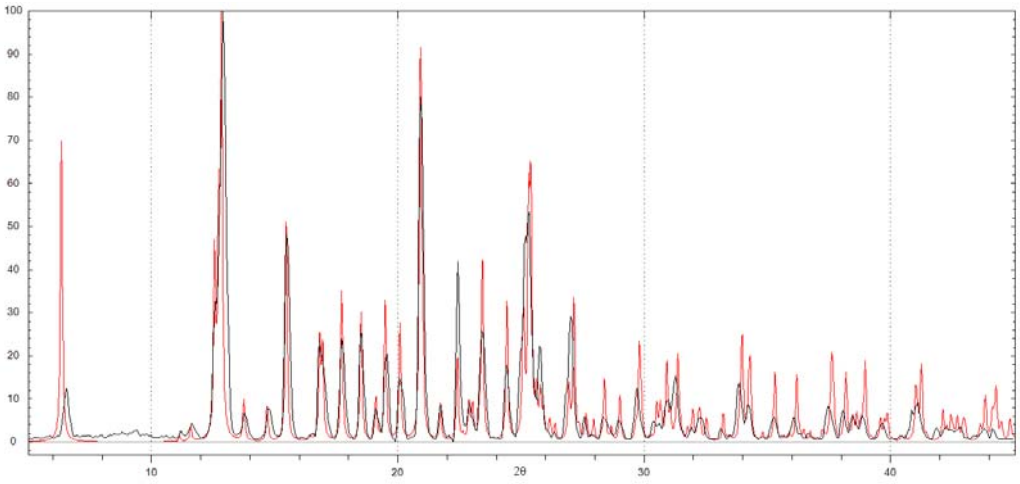

Fig. S1.5 Experimental powder pattern of **4-pnZnI** compared with the powder pattern calculated from the single crystal structure.

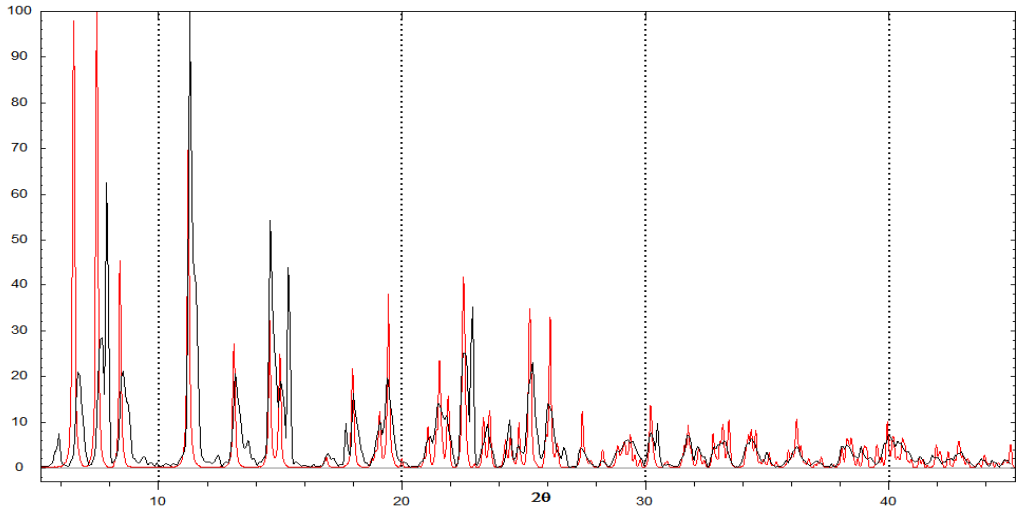

Fig. S1.6 Experimental powder pattern of **4-pnHgI** compared with the powder pattern calculated from the single crystal structure.

Section 2: Selected bond lengths, angles and other geometric parameters.

Table S2.1 Selected bond lengths, angles and torsion angles for complexes containing organic ligand **4-pn** (Å, °).

	4-pnCoCl M=Co, X=Cl	**4-pnCoBr** M=Co, X=Br	**4-pnZnBr** M=Zn, X=Br	**4-pnZnI** M=Zn, X=I	**4-pnHgI** M=Hg, X=I
M(1)-N(1) (Å)	2.063(4)	2.046(2)	2.0659(18)	2.066(4)	2.410(3)
M(1)-N(3) (Å)	-	-	-	-	2.410(3)
M(1)-X(1) (Å)	2.2547(14)	2.3715(4)	2.3552(3)	2.5488(5)	2.6762(3)
M(1)-X(2) (Å)	-	-	-	-	2.6942(3)
N(1)-M(1)-N(3) (°)	-	-	-	-	118.76(11)
N(1)^{i}-M(1)-N(1)	125.1(3)	95.91(14)	93.80(10)	93.8(2)	-
N(1)-M(1)-X(1) (°)	99.82(12)	104.36(6)	115.20(5)	114.50(10)	100.15(7)
N(3)-M(1)-X(1) (°)	-	-	-	-	99.73(7)
N(1)^{i}-M(1)-X(1)	102.20(12)	116.30(6)	104.30(5)	106.08(10)	-
N(1)-M(1)-X(2) (°)	-	-	-	-	95.68(7)
N(3)-M(1)-X(2) (°)	-	-	-	-	96.32(7)
N(1)-M(1)-X(1)^{i}	102.20(12)	104.36(4)	104.30(5)	106.08(10)	-
N(1)^{i}-M(1)-X(1)^{i}	99.82(12)	116.31(4)	115.20(5)	114.49(10)	-
X(1)-M(1)-X(1)^{i}	131.02(10)	117.87(3)	121.02(2)	119.17(4)	-
X(1)-M(1)-X(2) (°)	-	-	-	-	148.351(11)
N(2)-C(6)-C(3) (°)	111.9(5)	111.1(2)	111.09(17)	110.9(4)	111.2(3)
N(4)-C(24)-C(21) (°)	-	-	-	-	114.8(3)
C(17)-N(2)-C(6)-C(3) (°)	88.0(5)	90.3(3)	-86.7(2)	87.4(5)	-92.4(4)
C(7)-N(2)-C(6)-C(3) (°)	-92.6(6)	-86.2(3)	89.7(2)	-89.7(5)	86.6(4)
C(25)-N(4)-C(24)-C(21) (°)	-	-	-	-	86.4(4)
C(35)-N(4)-C(24)-C(21) (°)	-	-	-	-	-93.7(4)

i : -x,y,-z+1/2

Section 3: Complex Molecules

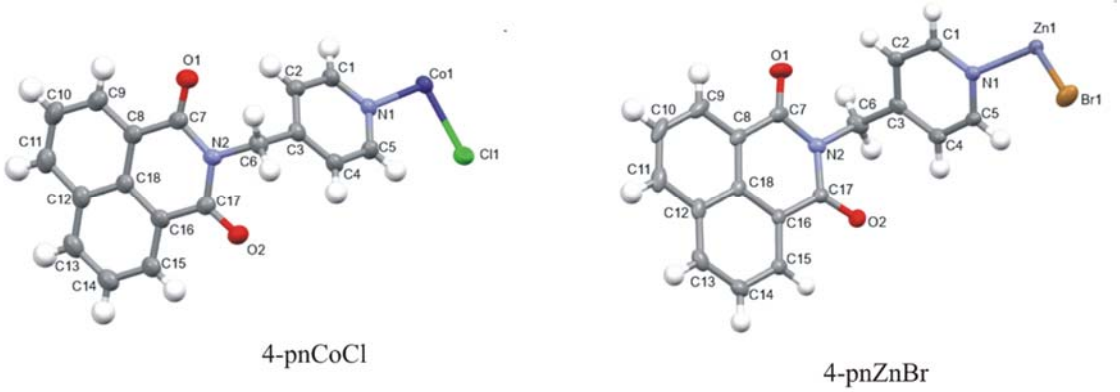

Figure S3.1 The asymmetric units of the structures **4-pnCoCl** and **4-pnZnBr** (also a representative of the asymmetric unit of the isostructural complexes **4-pnCoBr** and **4-pnZnI**), illustrating the atomic numbering scheme. Ellipsoids are drawn at the 50% probability level.

References:

1. F. R. Allen, *Acta Crystallogr., Sect. B: Struct. Sci*., 58, 380 (2002).
2. R. J. Sarma, C. Tamuly, M. N. Barooah and J. B. Baruah, *J. Mol. Struct*., 829, 29 (2007).