Supplementary Material for

Modulation of coordination in pincer-type isonicotinohydrazone Schiff base ligands by proton transfer

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Table S1 Hydrogen bonds geometry for **1** and **2**.

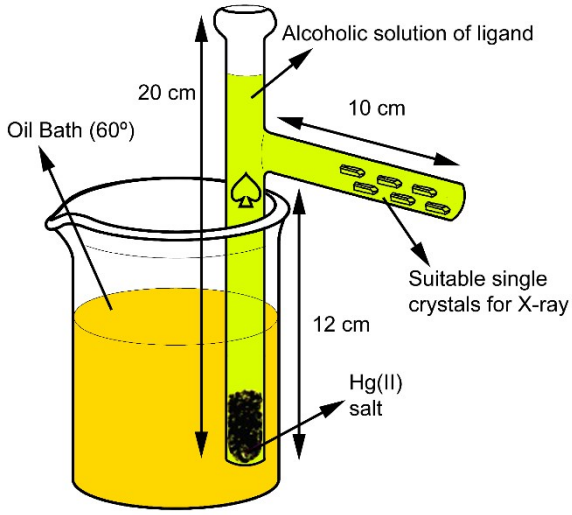
Crystal	D–H…A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
1	N1–H1…N4^{i}	0.86	2.220(7)	2.9258(7)	139.2(6)
	C11–H11…N6^{ii}	0.93	2.59(1)	3.434(9)	151.3(8)
	C12–H12…S2^{iii}	0.93	2.925(8)	3.649(8)	135.8(7)
2	N4–H4…N6^{iv}	0.86	1.975(4)	2.803(4)	161.2(3)
	C5–H5…N5^{v}	0.93	2.596(5)	3.324(5)	135.6(3)
	C9–H9…S2^{vi}	0.93	2.987(3)	3.864(3)	157.9(3)

Symmetry operation codes: ^{i} 1/2-*x*,1/2+*y*,1/2-*z*; ^{ii} 1/2-*x*,-1/2+*y*,1/2-*z*; ^{iii} *x*,2-*y*,1/2+*z*; ^{iv} 1+*x*,*y*,*z*; ^{v} *x*,1/2-*y*,-1/2+*z*; ^{vi} 2-*x*,-1/2+*y*, 1,5-*z*.

Table S2. Geometry of classical π…π interactions in **1** and **2**.

Crystal	π…π interaction	φ	Cg…Cg	Δ
1	R1…R1^{i}	0	3.655(6)	1.513(11)
	R2…R3^{ii}	13.8(3)	3.882(4)	1.563(13)
2	R1…R2^{iii}	9.8(1)	3.742(2)	1.523(5)

Angles in deg, distances in Å. φ – Angle between planes of interacting rings; Cg…Cg – centroid-centroid distance; Δ – shift between ring centroids. R1: N3-C3-C4-C5-C6-C7; R2: C8-C9-C10-N4-C11-C12; R3: C13-C14-C15-C16-C17-C18. Symmetry codes: ^{i} -*x*,1-*y*,1-*z*; ii 1/2-*x*,-1/2+*y*,1/2-*z*; ^{iii} 1-*x*,-*y*,-*z*.



Scheme. S1. Representation of the branched tube used for the crystallization of compounds **1**–**2**.

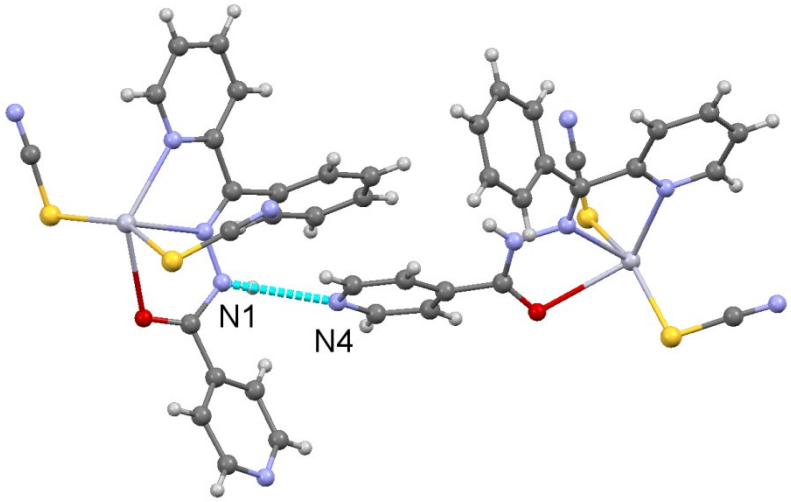


Fig. S1. N_{amide}–H…N Hydrogen bond in **1**.

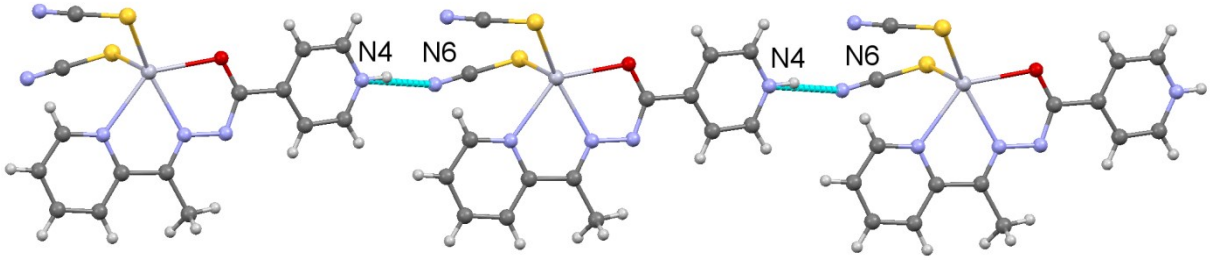


Fig. S2. $N_{pyridine}$–H…N Hydrogen bond in **2**.