

Supplementary data for the article:

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Supporting Information

Synthesis, characterization and antimicrobial activity of pentagonal-bipyramidal isothiocyanato Co(II) and Ni(II) complexes with 2,6-diacetylpyridine bis(trimethylammoniumacetohydrazone)

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Figure S3. Fragment of the crystal structure of $[\text{NiH}_2\text{L}(\text{NCS})_2](\text{SCN})_2$ showing hydrogen bonding interactions between complex ion and non-coordinated SCN^- anions.

Figure S4. Perspective view of complex cations $[\text{M}(\text{H}_2\text{L})(\text{NCS})_2]^{2+}$ (M = Co(II) and Ni(II)) forming dimers by means of intermolecular interactions of C–H \cdots π type in the crystals of isostructural $[\text{CoH}_2\text{L}(\text{NCS})_2](\text{SCN})_2$ and $[\text{NiH}_2\text{L}(\text{NCS})_2](\text{SCN})_2$ complexes.

Table S1. Hydrogen bonding geometry for $[\text{CoH}_2\text{L}(\text{NCS})_2](\text{SCN})_2$, $[\text{CoH}_2\text{L}(\text{NCS})_2][\text{Co}(\text{NCS})_4]$ and $[\text{NiH}_2\text{L}(\text{NCS})_2](\text{SCN})_2$.

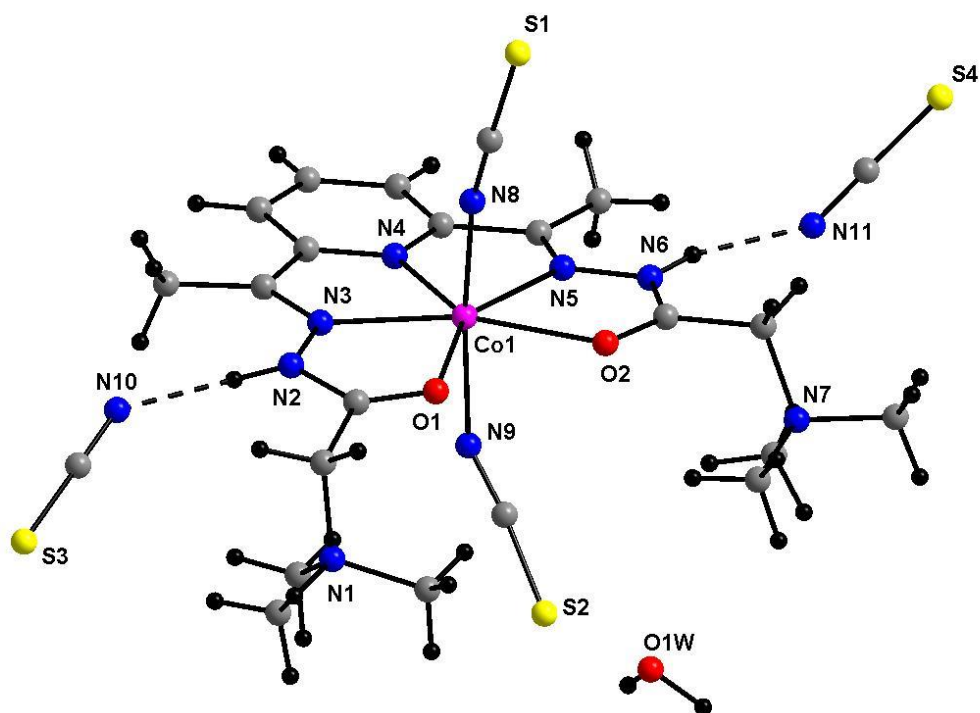


Figure S1. Fragment of the crystal structure of $[\text{CoH}_2\text{L}(\text{NCS})_2](\text{SCN})_2$ showing hydrogen bonding interactions between complex ion and non-coordinated SCN^- anions.

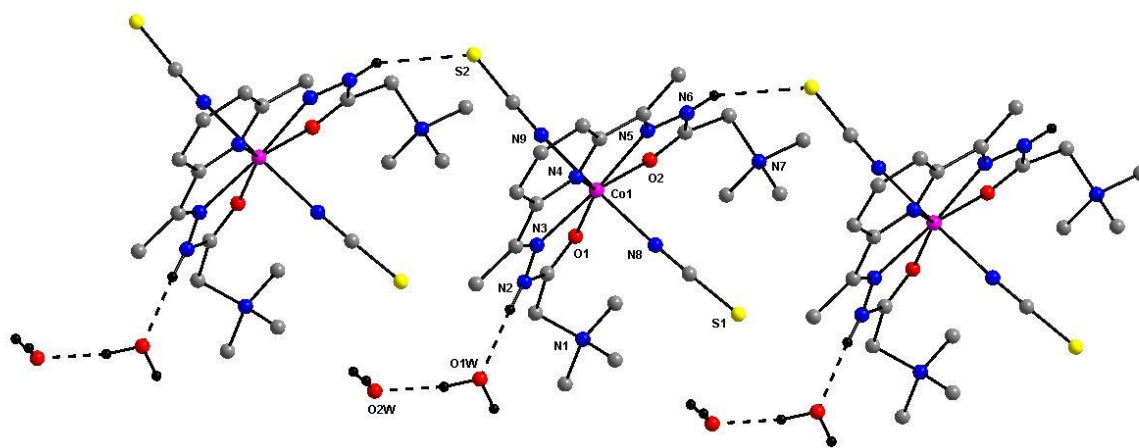


Figure S2. Fragment of the crystal structure of $[\text{CoH}_2\text{L}(\text{NCS})_2][\text{Co}(\text{NCS})_4]$ showing N–H \cdots S, N–H \cdots O and O–H \cdots O hydrogen bonding interactions between complex ions and non-coordinated water molecules. Hydrogen atoms not involved in hydrogen bonding and $[\text{Co}(\text{NCS})_4]^{2-}$ anions have been removed for clarity.

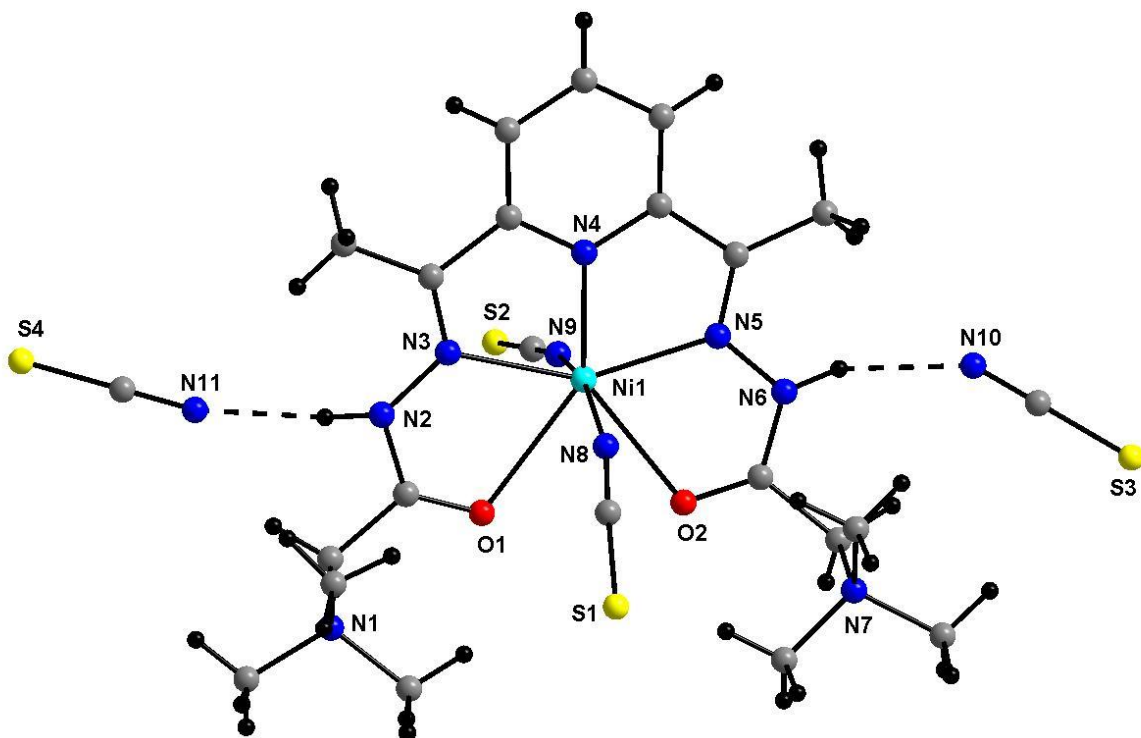


Figure S3. Fragment of the crystal structure of $[\text{NiH}_2\text{L}(\text{NCS})_2](\text{SCN})_2$ showing hydrogen bonding interactions between complex ion and non-coordinated SCN^- anions.

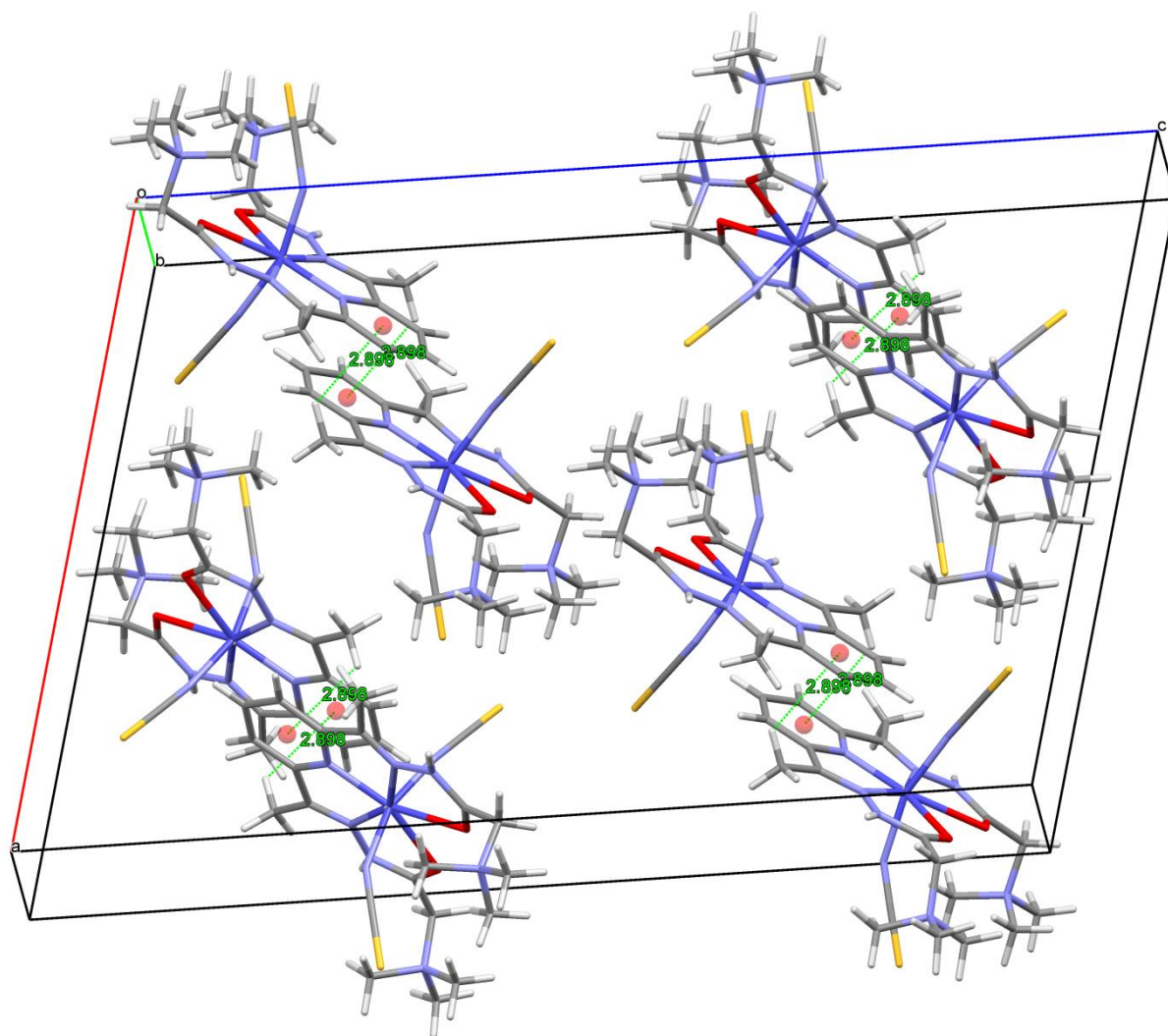


Figure S4. Perspective view of complex cations $[M(\text{H}_2\text{L})(\text{NCS})_2]^{2+}$ ($M = \text{Co}(\text{II})$ and $\text{Ni}(\text{II})$) forming dimers by means of intermolecular interactions of $\text{C}-\text{H}\cdots\pi$ type in the crystals of isostructural $[\text{CoH}_2\text{L}(\text{NCS})_2](\text{SCN})_2$ and $[\text{NiH}_2\text{L}(\text{NCS})_2](\text{SCN})_2$ complexes.

Table S1. Hydrogen bonding geometry for $[\text{CoH}_2\text{L}(\text{NCS})_2](\text{SCN})_2$, $[\text{CoH}_2\text{L}(\text{NCS})_2][\text{Co}(\text{NCS})_4]$ and $[\text{NiH}_2\text{L}(\text{NCS})_2](\text{SCN})_2$.

D – H ... A	$d(\text{D} - \text{H})/\text{Å}$	$d(\text{H} \cdots \text{A})/\text{Å}$	$d(\text{D} \cdots \text{A})/\text{Å}$	$\angle(\text{DHA})/\text{°}$	Symmetry transformation for acceptors
$[\text{CoH}_2\text{L}(\text{NCS})_2](\text{SCN})_2$					
N2–H2N...N10	0.887(19)	1.99(3)	2.844(5)	161(5)	x, y-1, z
N6–H6N...N11	0.88(2)	1.98(3)	2.830(8)	162(6)	-x+2, y+1/2, -z+1/2
$[\text{CoH}_2\text{L}(\text{NCS})_2][\text{Co}(\text{NCS})_4]$					
N2–H2N...O1w	0.87(2)	1.96(3)	2.748(7)	151(5)	
N6–H6N...S2	0.88(2)	2.66(3)	3.469(5)	154(6)	x, y+1, z
O1w–H1w...O2w	0.95(2)	1.78(3)	2.724(9)	168(9)	x-1/2, -y+1/2, z+1/2
$[\text{NiH}_2\text{L}(\text{NCS})_2](\text{SCN})_2$					
N2–H2N...N11	0.864(19)	1.98(2)	2.838(5)	174(5)	x-1/2, -y+1, z
N6–H6N...N10	0.898(18)	2.03(2)	2.881(4)	157(4)	x, y-1, z