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interactions; Hirshfeld surface analysis.**CCDC references:** 1979499; 1979498**Supporting information:** this article has
supporting information at journals.iucr.org/e

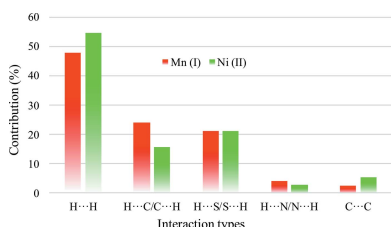
Crystal structures and Hirshfeld surface analysis of *trans*-bis(thiocyanato- κN)bis[2,4,6-trimethyl-*N*-[(pyridin-2-yl)methylidene]aniline- $\kappa^2 N, N'$]manganese(II) and *trans*-bis(thiocyanato- κN)bis[2,4,6-trimethyl-*N*-[(pyridin-2-yl)methylidene]aniline- $\kappa^2 N, N'$]nickel(II)

Siripak Jittirattanakun,^a Chatphorn Theppitak,^a Nanthawat Wannarit,^a Bachari Rotsut^b and Kittipong Chainok^{c*}^aDivision of Chemistry, Faculty of Science and Technology, Thammasat University, Khlong Luang, Pathum Thani, 12121, Thailand, ^bWisetchaichan Tantiwittayapoom School, Wisetchaichan, Angthong, 14110, Thailand, and ^cMaterials and Textile Technology, Faculty of Science and Technology, Thammasat University, Khlong Luang, Pathum Thani, 12121, Thailand. *Correspondence e-mail: kc@tu.ac.th

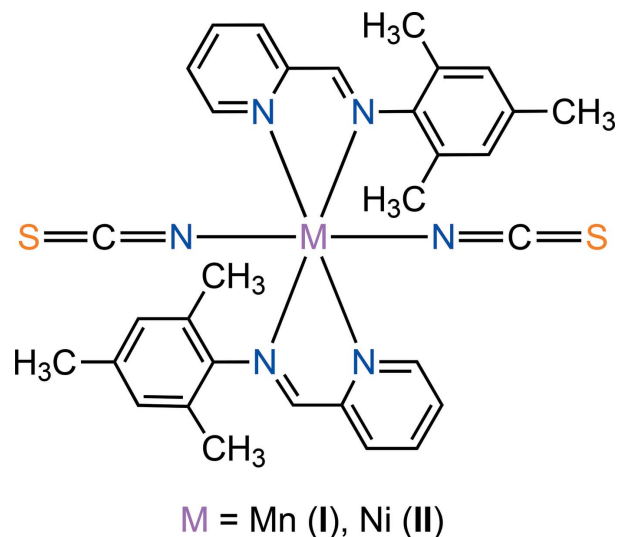
Two new mononuclear metal complexes involving the bidentate Schiff base ligand 2,4,6-trimethyl-*N*-[(pyridin-2-yl)methylidene]aniline (C₁₅H₁₆N₂ or PM-TMA), [Mn(NCS)₂(PM-TMA)₂] (**I**) and [Ni(NCS)₂(PM-TMA)₂] (**II**), were synthesized and their structures determined by single-crystal X-ray diffraction. Although the title compounds crystallize in different crystal systems [triclinic for (**I**) and monoclinic for (**II**)], both asymmetric units consist of one-half of the complex molecule, *i.e.* one metal(II) cation, one PM-TMA ligand, and one N-bound thiocyanate anion. In both complexes, the metal(II) cation is located on a centre of inversion and adopts a distorted octahedral coordination environment defined by four N atoms from two symmetry-related PM-TMA ligands in the equatorial plane and two N atoms from two symmetry-related NCS[−] anions in a *trans* axial arrangement. The trimethylbenzene and pyridine rings of the PM-TMA ligand are oriented at dihedral angles of 74.18 (7) and 77.70 (12)° for (**I**) and (**II**), respectively. The subtle change in size of the central metal cations leads to a different crystal packing arrangement for (**I**) and (**II**) that is dominated by weak C—H...S, C—H... π , and π — π interactions. Hirshfeld surface analysis and two-dimensional fingerprint plots were used to quantify these intermolecular contacts, and indicate that the most significant contacts in packing are H...H [48.1% for (**I**) and 54.9% for (**II**)], followed by H...C/C...H [24.1% for (**I**) and 15.7% for (**II**)], and H...S/S...H [21.1% for (**I**) and 21.1% for (**II**)].

1. Chemical context

Schiff bases are widely employed as ligands in the development of coordination chemistry (Liu & Hamon, 2019). Among them, derivatives of the Schiff base 2-pyridylmethanimine have been used as chelating ligands in the construction of discrete metal complexes exhibiting interesting luminescent properties (Basu Baul *et al.*, 2013), magnetic spin-crossover behaviour (Létard *et al.*, 1997; Capes *et al.*, 2000), or biological and catalytic reactivities (Cozzi, 2004; Creaven *et al.*, 2010). These ligands are also able to generate non-covalent interactions such as hydrogen bonding and π — π stacking that aid in stabilizing the assembly and provide diversity to the architectures of the crystal structures. On the other hand, pseudohalides such as thiocyanate (NCS[−]) and selenocyanate



(NCS[−]) anions are a class of rigid ligands with either a terminal or a bridging coordination behaviour. They have been employed extensively with neutral *N*-donor co-ligands in the development of novel functional coordination magnets materials, particularly in the field of molecular-based magnets (Suckert *et al.*, 2016).



In this work, we combined 2-pyridinecarboxaldehyde and 2,4,6-trimethylaniline to synthesize a new bidentate Schiff base ligand with two potential *N,N'*-donor sites, *viz.* 2,4,6-trimethyl-*N*-[(pyridin-2-yl)methylidene]aniline (C₁₅H₁₆N₂ or PM-TMA). Reaction of the PM-TMA ligand and *M*(NCS)₂ precursors (*M* = Mn, Ni) in methanolic solutions resulted in the formation of discrete mononuclear complexes with the formula [*M*(NCS)₂(PM-TMA)₂], *M* = Mn (**I**), Ni (**II**). Their molecular and crystal structures as well as Hirshfeld surface analysis are reported.

2. Structural commentary

The molecular structures of (**I**) and (**II**) are shown in Fig. 1 and 2. Although the title compounds crystallize in different space groups [*P*1̄ for (**I**) and *P*2₁/*n* for (**II**)], in both cases the

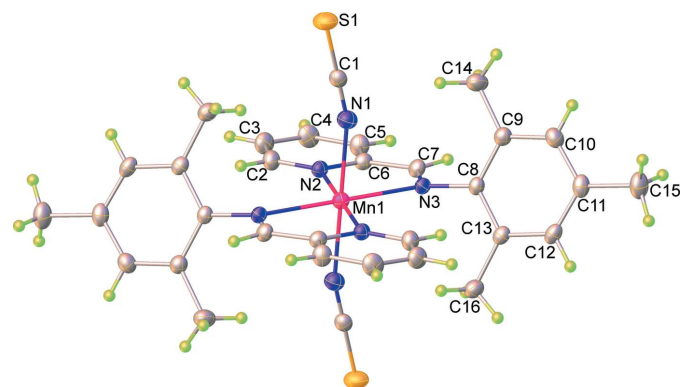


Figure 1
Molecular structures of the title complex (**I**), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

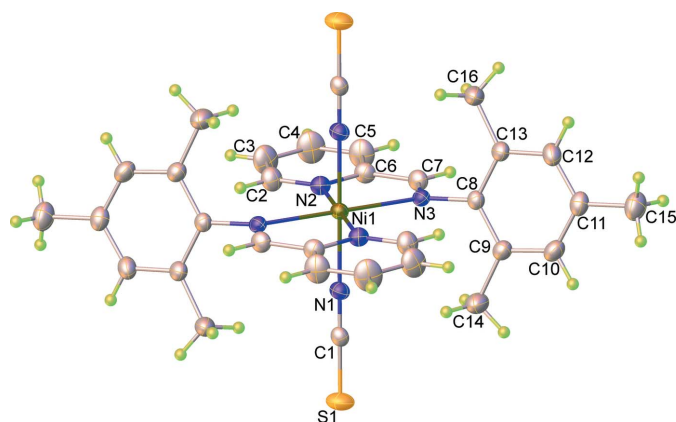


Figure 2
Molecular structures of the title complex (**II**), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

asymmetric unit consist of one-half of the molecule, *i.e.* one metal(II) cation, one PM-TMA ligand and one thiocyanate anion. Each metal(II) cation is located on a centre of inversion and adopts a distorted octahedral coordination environment with four N atoms from two symmetry-related PM-TMA ligands in the equatorial plane and two N atoms from symmetry-related NCS[−] anions in a *trans* axial arrangement. The *M*–N bond lengths [2.174 (2) to 2.312 (2) Å for (**I**) and 2.027 (3) to 2.184 (2) Å for (**II**)] and N–*M*–N bond angles [74.27 (6) to 180° for (**I**) and 78.4 (1) to 180° for (**II**)] for both complexes are all in the normal range for similar Schiff base complexes with Mn^{II} (Chattopadhyay *et al.*, 2002; Lucas *et al.*, 2005) and Ni^{II} (Guo, 2009; Layek *et al.*, 2014) ions. Note that the Mn1–N1–C1 bond angle [164.3 (2)°] in (**I**) is somewhat more bent than the corresponding Ni1–N1–C1 bond angle [176.7 (3)°] in (**II**). The PM-TMA ligands are not co-planar, with the trimethylbenzene ring oriented to the pyridine ring at a dihedral angle of 74.18 (7) and 77.70 (12)° for (**I**) and (**II**), respectively. An overlay of the complex molecules of (**I**) and (**II**) is illustrated in Fig. 3, showing the slight differences in orientation of the trimethylbenzene rings and thiocyanate anions. This impacts significantly upon the molecular packing as described in the next section.

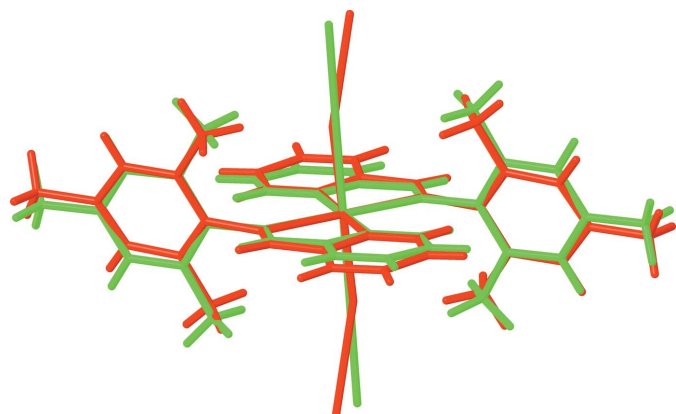


Figure 3
View of the structure overlay of (**I**) (red) and (**II**) (green).

Table 1
Hydrogen-bond geometry (Å, °) for **(I)**.

Cg1 is the mid-point of the C1=N1 group. Cg2 and Cg3 are the centroids of the N2/C2–C6 and C8–C13 rings.

<i>D</i> –H... <i>A</i>	<i>D</i> –H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> –H... <i>A</i>
C3–H3...S1 ⁱ	0.93	3.16	3.812 (3)	129
C4–H4...Cg1 ⁱ	0.93	2.89	3.561 (3)	129
C5–H5...S1 ⁱⁱ	0.93	3.00	3.785 (3)	143
C7–H7...S1 ⁱⁱ	0.93	3.07	3.871 (2)	146
C14–H14A...Cg1 ⁱⁱ	0.96	2.89	3.779 (3)	153
C14–H14B...Cg2 ⁱⁱ	0.96	2.68	3.556 (3)	152
C16–H16C...Cg3 ⁱⁱⁱ	0.96	3.14	3.711 (3)	145

Symmetry codes: (i) $x, y + 1, z$; (ii) $-x, -y + 1, -z + 1$; (iii) $-x + 1, -y + 1, -z + 2$.

3. Supramolecular features

The crystal packing of **(I)** and **(II)** is dominated by weak C–H...S, C–H... π , and π – π interactions. In the crystal structure of **(I)**, pairs of weak C–H...S hydrogen bonds along with the C–H... π interactions involving the methyl H atoms (H14A and H14B) and the trimethylbenzene ring or the midpoint of thiocyanate C=N group, Table 1, link inversion-related molecules into a chain running parallel to the *a* axis, Fig. 4. The chains are further linked into a three-dimensional

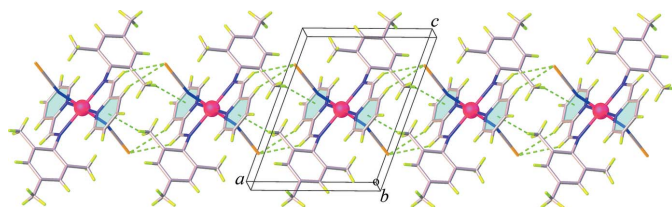


Figure 4
View of chains in **(I)** generated through C–H...S and C–H... π interactions.

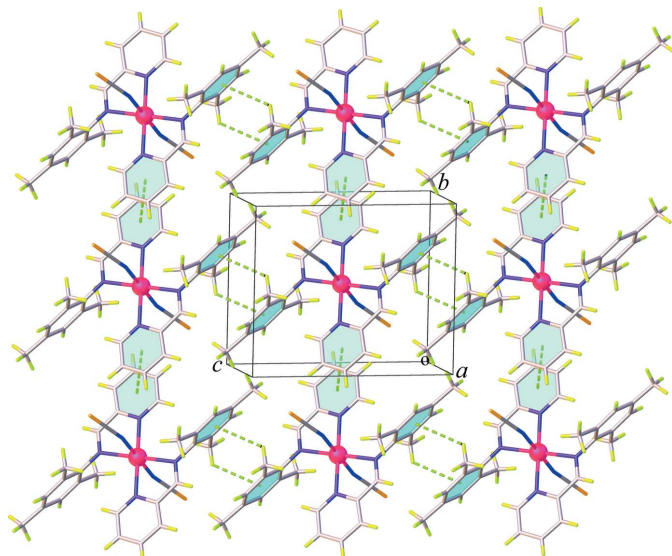


Figure 5
View of the three-dimensional network in **(I)** generated through C–H... π and π – π interactions.

Table 2
Hydrogen-bond geometry (Å, °) for **(II)**.

Cg1 is the mid-point of the C1=N1 group.

<i>D</i> –H... <i>A</i>	<i>D</i> –H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> –H... <i>A</i>
C4–H4...S1 ⁱ	0.93	2.89	3.769 (4)	158
C7–H7...S1 ⁱⁱ	0.93	2.83	3.680 (3)	153
C10–H10...S1 ⁱⁱⁱ	0.93	3.17	3.871 (4)	134
C10–H10...Cg1 ⁱⁱⁱ	0.93	2.73	3.655 (4)	171

Symmetry codes: (i) $x + 1, y, z$; (ii) $x + \frac{1}{2}, -y + \frac{3}{2}, z - \frac{1}{2}$; (iii) $x - \frac{1}{2}, -y + \frac{3}{2}, z - \frac{1}{2}$.

supramolecular network through weak π – π interactions involving the pyridine rings [centroid-to-centroid distance = 3.909 (3) Å] and additional weak C–H... π interactions

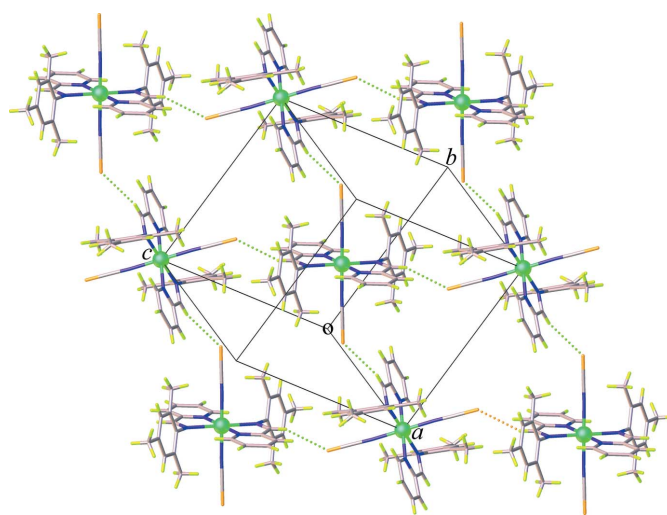


Figure 6
Formation of a two-dimensional supramolecular network in **(II)** generated through C–H...S hydrogen bonds.

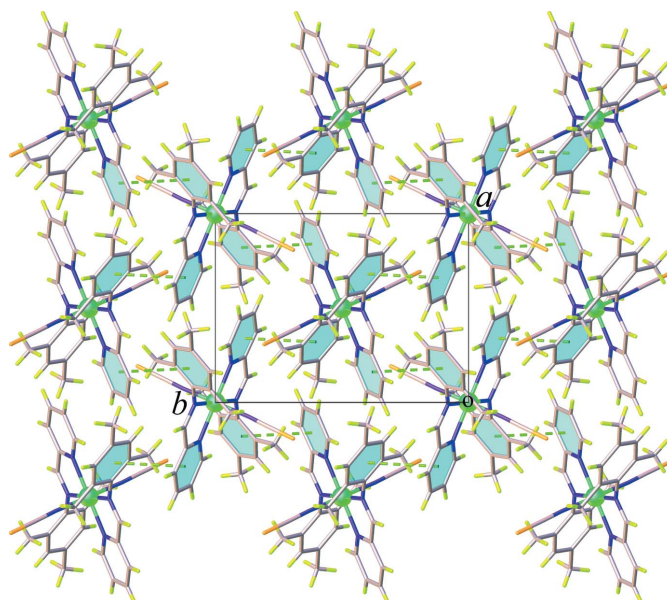


Figure 7
Crystal packing of **(II)** viewed along the *c* axis with aromatic π – π stacking interactions bonds shown as dashed lines.

between the methyl H atoms and the trimethylbenzene rings, Fig. 5 (Table 1). For **(II)**, adjacent molecules are linked together into a sheet extending parallel to (101), Fig. 6, by weak C—H···S hydrogen bonds between the methine C—H groups and the thiocyanate S atoms, Table 2. On the other hand, as seen in Fig. 7, the packing in **(II)** also features weak π – π stacking interactions arising from the pyridine rings and the trimethylbenzene rings [centroid-to-centroid distance = 4.147 (3) Å, dihedral angle = 17.41 (14)°]. There is an additional C—H··· π interaction between the methyl H atom and the midpoint of the thiocyanate C=N group (Table 2). These interactions help to enhance the dimensionality into a three-dimensional supramolecular architecture.

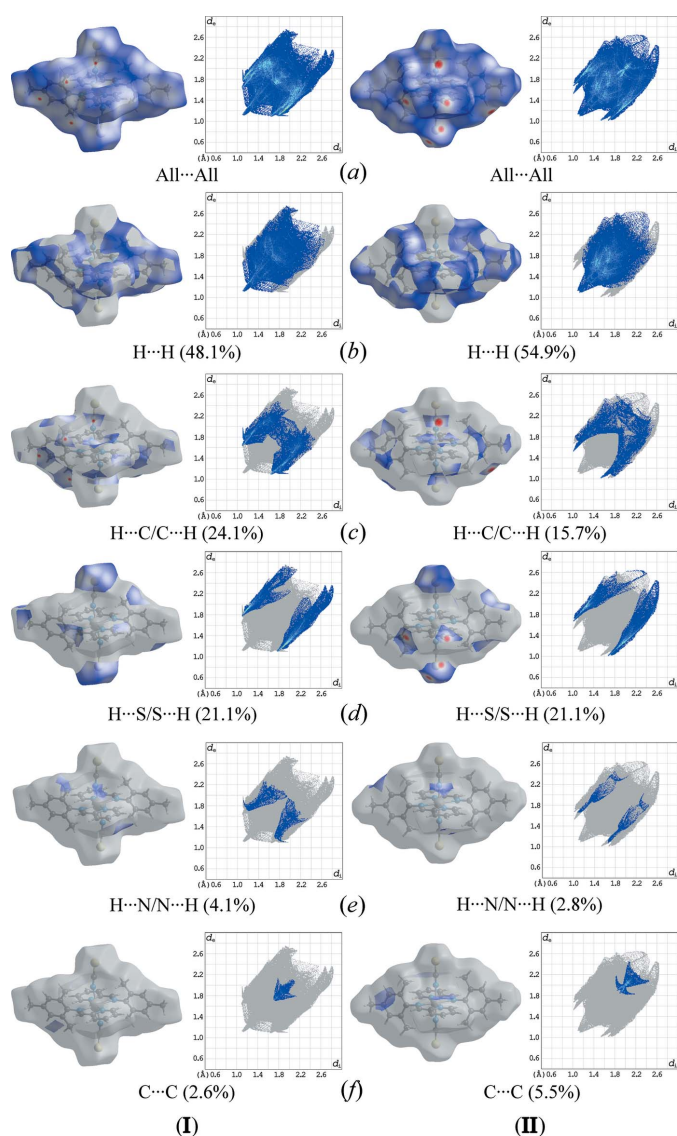


Figure 8

Two-dimensional fingerprint plots of **(I)** and **(II)**, showing (a) all interactions, and those delineated into (b) H···H, (c) H···C/C···H, (d) H···S/S···H, (e) H···N/N···H, and (f) C···C contacts [d_e and d_i represent the distances from a point on the Hirshfeld surface to the nearest atoms outside (external) and inside (internal) the surface, respectively].

4. Hirshfeld surface analysis

The intermolecular interactions between the molecules in the crystal structures of **(I)** and **(II)** were quantified by Hirshfeld surface analysis (McKinnon *et al.*, 2007) and two-dimensional fingerprint plots (Spackman & McKinnon, 2002) generated by *CrystalExplorer* (Turner *et al.*, 2017); results are shown in Figs. 8 and 9, respectively. Major contributions to the d_{norm} surfaces in both cases are H···H contacts [48.1% for **(I)** and 54.9% for **(II)**], which represent van der Waals interactions. Minor contributions are due to H···C/C···H [24.1% for **(I)** and 15.7% for **(II)**] and H···S/S···H (21.1% for **(I)** and 21.1% for **(II)**) contacts, associated with weak C—H··· π and C—H···S interactions, respectively. These contributions are characterized as bright-red spots on the Hirshfeld surface mapped over d_{norm} and are observed as two sharp peaks in the two-dimensional plots. The C···C contacts associated with aromatic π – π stacking contribute only with a small percentage in **(I)** (2.6%) and about twice the amount in **(II)** (5.5%). H···N/N···H contacts in both cases are negligible.

5. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.40, last update August 2019; Groom *et al.*, 2016) revealed no match for coordination compounds with the Schiff base 2,4,6-trimethyl-*N*-[(pyridin-2-yl)methylidene]aniline. A general search for thiocyanato coordination compounds involving transition metals and *N*-[(pyridin-2-yl)methylidene]aniline as the main skeleton resulted in 122 structures with different substituents on the benzyl rings. In these structures, the two bidentate Schiff base ligands and the two thiocyanate anions are octahedrally arranged around the central metal cations in a *cis*-conformation. There is only one complex with a *trans*-conformation and the same skeleton as in the title complexes, *viz.* *trans*-[Cd(NCS)₂(C₁₄H₁₄N₂)₂] (CSD refcode GARTAW; Malekshahian *et al.*, 2012). In this complex, weak C—H···S hydrogen bonds consolidate the crystal packing, similar to the title complexes **(I)** and **(II)**.

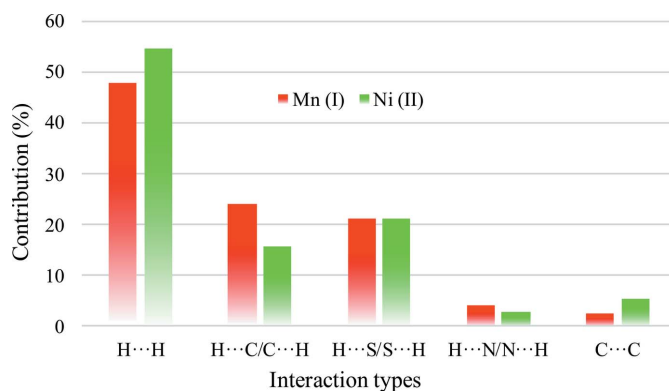


Figure 9

Quantitative results of different intermolecular contacts contributing to the Hirshfeld surfaces of **(I)** and **(II)**.

Table 3
Experimental details.

	(I)	(II)
Crystal data		
Chemical formula	[Mn(NCS) ₂ (C ₁₅ H ₁₆ N ₂) ₂]	[Ni(NCS) ₂ (C ₁₅ H ₁₆ N ₂) ₂]
<i>M_r</i>	619.69	623.46
Crystal system, space group	Triclinic, <i>P</i> $\bar{1}$	Monoclinic, <i>P</i> 2 ₁ / <i>n</i>
Temperature (K)	296	296
<i>a</i> , <i>b</i> , <i>c</i> (Å)	8.5597 (5), 9.0255 (5), 10.7718 (7)	9.6156 (5), 12.6786 (7), 12.9870 (7)
α , β , γ (°)	91.718 (2), 109.830 (2), 95.080 (2)	90, 101.250 (2), 90
<i>V</i> (Å ³)	778.16 (8)	1552.85 (14)
<i>Z</i>	1	2
Radiation type	Mo <i>K</i> α	Mo <i>K</i> α
μ (mm ⁻¹)	0.59	0.79
Crystal size (mm)	0.28 × 0.28 × 0.22	0.34 × 0.3 × 0.3
Data collection		
Diffractometer	Bruker D8 QUEST CMOS PHOTON II	Bruker D8 QUEST CMOS PHOTON II
Absorption correction	Multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015)	Multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015)
<i>T</i> _{min} , <i>T</i> _{max}	0.673, 0.745	0.607, 0.745
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	7594, 3091, 2326	16977, 3037, 2486
<i>R</i> _{int}	0.043	0.032
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.625	0.618
Refinement		
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> [<i>F</i> ²], <i>S</i>	0.044, 0.100, 1.02	0.053, 0.104, 1.21
No. of reflections	3091	3037
No. of parameters	190	190
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å ⁻³)	0.27, -0.20	0.70, -0.47

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015a), *SHELXL* (Sheldrick, 2015b) and *OLEX2* (Dolomanov *et al.*, 2009).

6. Synthesis and crystallization

All reagents were of analytical grade and were used as received without further purification. The bidentate Schiff base ligand, 2,4,6-trimethyl-*N*-[(pyridin-2-yl)methylidene]aniline (C₁₅H₁₆N₂ or PM-TMA) was synthesized according to a literature method (Theppitak *et al.*, 2014). A solution of PM-TMA (89.7 mg, 0.4 mmol) in methanol (5 ml) was placed in a test tube. To a solution of Mn(ClO₄)₂·6H₂O (50.8 mg, 0.2 mmol) in methanol (5 ml) was added KNCS (39.0 mg, 0.4 mmol), and the solution was stirred at room temperature for 30 min and then filtered to remove a white precipitate of KClO₄. The solution was then carefully layered on the methanol solution of PM-TMA. After slow diffusion at room temperature for 3 d, yellow block-shaped crystals of (I) were obtained in 88% yield (44.7 mg) based on the manganese(II) source. Complex (II) was prepared following the procedure described above for (I), except that Ni(ClO₄)₂·6H₂O (58.2 mg, 0.2 mmol) and KNCS (39.0 mg, 0.4 mmol) were used. Yellow block-shaped crystal of (II) were obtained in 82% yield (47.7 mg) based on the nickel(II) source.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All C-bound H atoms were placed in calculated positions and refined using a riding model with C—H = 0.93–0.97 Å and with *U*_{iso}(H) = 1.2–1.5*U*_{eq}(C).

Acknowledgements

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supporting information

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Crystal structures and Hirshfeld surface analysis of *trans*-bis(thiocyanato- κ N)bis{2,4,6-trimethyl-*N*-[(pyridin-2-yl)methylidene]aniline- κ^2 N,N'}manganese(II) and *trans*-bis(thiocyanato- κ N)bis{2,4,6-trimethyl-*N*-[(pyridin-2-yl)methylidene]aniline- κ^2 N,N'}nickel(II)

Siripak Jittirattanakun, Chatphorn Theppitak, Nanthawat Wannarit, Bachari Rotsut and Kittipong Chainok

Computing details

For both structures, data collection: *APEX3* (Bruker, 2016); cell refinement: *SAINT* (Bruker, 2016); data reduction: *SAINT* (Bruker, 2016); program(s) used to solve structure: *ShelXT* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015b); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

***trans*-Bis(thiocyanato- κ N)bis{2,4,6-trimethyl-*N*-[(pyridin-2-yl)methylidene]aniline- κ^2 N,N'}manganese(II) (1)**

Crystal data

[Mn(NCS)₂(C₁₅H₁₆N₂)₂]

$M_r = 619.69$

Triclinic, $P\bar{1}$

$a = 8.5597$ (5) Å

$b = 9.0255$ (5) Å

$c = 10.7718$ (7) Å

$\alpha = 91.718$ (2)°

$\beta = 109.830$ (2)°

$\gamma = 95.080$ (2)°

$V = 778.16$ (8) Å³

$Z = 1$

$F(000) = 323$

$D_x = 1.322$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2271 reflections

$\theta = 2.9$ – 25.8 °

$\mu = 0.59$ mm⁻¹

$T = 296$ K

Block, yellow

$0.28 \times 0.28 \times 0.22$ mm

Data collection

BRUKER D8 QUEST CMOS PHOTON II
diffractometer

Radiation source: sealed x-ray tube

Graphite monochromator

Detector resolution: 7.39 pixels mm⁻¹

φ and ω scans

Absorption correction: multi-scan
(*SADABS*; Krause *et al.*, 2015)

$T_{\min} = 0.673$, $T_{\max} = 0.745$

7594 measured reflections

3091 independent reflections

2326 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.043$

$\theta_{\max} = 26.4$ °, $\theta_{\min} = 2.9$ °

$h = -10 \rightarrow 10$

$k = -11 \rightarrow 11$

$l = -13 \rightarrow 13$

*Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.044$ $wR(F^2) = 0.100$ $S = 1.02$

3091 reflections

190 parameters

0 restraints

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0454P)^2 + 0.1287P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} < 0.001$ $\Delta\rho_{\max} = 0.27 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\min} = -0.20 \text{ e } \text{\AA}^{-3}$ *Special details*

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Mn1	0.500000	0.500000	0.500000	0.03059 (16)
S1	-0.00476 (8)	0.21358 (9)	0.19246 (7)	0.0556 (2)
N1	0.2655 (2)	0.3678 (2)	0.3908 (2)	0.0432 (5)
N2	0.3816 (2)	0.71929 (19)	0.47958 (17)	0.0305 (4)
N3	0.4064 (2)	0.5223 (2)	0.67669 (17)	0.0295 (4)
C1	0.1524 (3)	0.3041 (3)	0.3083 (2)	0.0352 (5)
C2	0.3662 (3)	0.8173 (3)	0.3873 (2)	0.0394 (6)
H2	0.403637	0.795727	0.317827	0.047*
C3	0.2972 (3)	0.9498 (3)	0.3898 (3)	0.0460 (6)
H3	0.286186	1.014330	0.322324	0.055*
C4	0.2457 (3)	0.9843 (3)	0.4924 (3)	0.0486 (7)
H4	0.200641	1.073625	0.496677	0.058*
C5	0.2609 (3)	0.8853 (3)	0.5905 (2)	0.0431 (6)
H5	0.226735	0.906801	0.661687	0.052*
C6	0.3284 (3)	0.7535 (2)	0.5801 (2)	0.0325 (5)
C7	0.3369 (3)	0.6414 (3)	0.6780 (2)	0.0340 (5)
H7	0.290036	0.657904	0.742805	0.041*
C8	0.3925 (3)	0.4146 (2)	0.7695 (2)	0.0301 (5)
C9	0.2353 (3)	0.3410 (3)	0.7554 (2)	0.0364 (5)
C10	0.2266 (3)	0.2367 (3)	0.8455 (2)	0.0415 (6)
H10	0.123433	0.186156	0.836340	0.050*
C11	0.3663 (3)	0.2049 (3)	0.9487 (2)	0.0403 (6)
C12	0.5191 (3)	0.2774 (3)	0.9573 (2)	0.0375 (6)
H12	0.614163	0.255307	1.024579	0.045*
C13	0.5366 (3)	0.3818 (2)	0.8697 (2)	0.0328 (5)
C14	0.0778 (3)	0.3699 (3)	0.6467 (3)	0.0531 (7)
H14A	0.041645	0.462049	0.667966	0.080*
H14B	-0.007793	0.289925	0.637957	0.080*
H14C	0.098935	0.376187	0.564940	0.080*
C15	0.3481 (4)	0.0982 (3)	1.0500 (3)	0.0573 (8)

H15A	0.456430	0.073952	1.103645	0.086*
H15B	0.280474	0.008835	1.005464	0.086*
H15C	0.295925	0.144197	1.105062	0.086*
C16	0.7065 (3)	0.4597 (3)	0.8867 (2)	0.0441 (6)
H16A	0.733250	0.440009	0.808518	0.066*
H16B	0.788622	0.423560	0.961442	0.066*
H16C	0.705757	0.565104	0.900840	0.066*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0319 (3)	0.0273 (3)	0.0335 (3)	0.0076 (2)	0.0113 (2)	0.0037 (2)
S1	0.0379 (4)	0.0659 (5)	0.0543 (4)	−0.0008 (3)	0.0070 (3)	−0.0082 (4)
N1	0.0384 (11)	0.0424 (13)	0.0473 (12)	0.0020 (10)	0.0131 (10)	0.0040 (10)
N2	0.0318 (10)	0.0278 (10)	0.0316 (10)	0.0050 (8)	0.0096 (8)	0.0048 (8)
N3	0.0300 (9)	0.0285 (10)	0.0294 (10)	0.0065 (8)	0.0084 (8)	0.0067 (8)
C1	0.0328 (12)	0.0352 (13)	0.0415 (14)	0.0094 (11)	0.0161 (11)	0.0071 (11)
C2	0.0447 (14)	0.0362 (14)	0.0399 (14)	0.0049 (11)	0.0170 (11)	0.0080 (11)
C3	0.0515 (15)	0.0363 (14)	0.0521 (16)	0.0106 (12)	0.0177 (13)	0.0171 (12)
C4	0.0556 (16)	0.0325 (14)	0.0646 (18)	0.0183 (12)	0.0251 (14)	0.0150 (12)
C5	0.0514 (15)	0.0372 (14)	0.0469 (15)	0.0149 (12)	0.0223 (12)	0.0058 (11)
C6	0.0329 (12)	0.0285 (12)	0.0348 (13)	0.0062 (10)	0.0091 (10)	0.0043 (10)
C7	0.0373 (12)	0.0367 (14)	0.0290 (12)	0.0084 (11)	0.0115 (10)	0.0022 (10)
C8	0.0360 (12)	0.0274 (12)	0.0291 (12)	0.0082 (10)	0.0126 (10)	0.0046 (9)
C9	0.0372 (12)	0.0377 (14)	0.0358 (13)	0.0097 (11)	0.0129 (10)	0.0060 (10)
C10	0.0425 (14)	0.0372 (14)	0.0498 (15)	0.0043 (11)	0.0220 (12)	0.0078 (12)
C11	0.0583 (16)	0.0299 (13)	0.0399 (14)	0.0116 (12)	0.0240 (12)	0.0072 (10)
C12	0.0465 (14)	0.0355 (13)	0.0299 (12)	0.0156 (12)	0.0095 (11)	0.0063 (10)
C13	0.0390 (12)	0.0299 (12)	0.0288 (12)	0.0088 (10)	0.0096 (10)	0.0015 (9)
C14	0.0353 (13)	0.0594 (18)	0.0598 (18)	0.0039 (13)	0.0092 (13)	0.0166 (14)
C15	0.078 (2)	0.0481 (17)	0.0577 (18)	0.0182 (15)	0.0347 (16)	0.0215 (14)
C16	0.0401 (13)	0.0474 (16)	0.0401 (14)	0.0053 (12)	0.0071 (11)	0.0077 (12)

Geometric parameters (Å, °)

Mn1—N1 ⁱ	2.174 (2)	C7—H7	0.9300
Mn1—N1	2.174 (2)	C8—C9	1.404 (3)
Mn1—N2 ⁱ	2.2856 (17)	C8—C13	1.398 (3)
Mn1—N2	2.2855 (17)	C9—C10	1.388 (3)
Mn1—N3	2.3118 (17)	C9—C14	1.505 (3)
Mn1—N3 ⁱ	2.3117 (17)	C10—H10	0.9300
S1—C1	1.624 (3)	C10—C11	1.387 (3)
N1—C1	1.160 (3)	C11—C12	1.382 (3)
N2—C2	1.332 (3)	C11—C15	1.514 (3)
N2—C6	1.346 (3)	C12—H12	0.9300
N3—C7	1.276 (3)	C12—C13	1.387 (3)
N3—C8	1.441 (3)	C13—C16	1.508 (3)
C2—H2	0.9300	C14—H14A	0.9600

C2—C3	1.383 (3)	C14—H14B	0.9600
C3—H3	0.9300	C14—H14C	0.9600
C3—C4	1.359 (4)	C15—H15A	0.9600
C4—H4	0.9300	C15—H15B	0.9600
C4—C5	1.384 (3)	C15—H15C	0.9600
C5—H5	0.9300	C16—H16A	0.9600
C5—C6	1.386 (3)	C16—H16B	0.9600
C6—C7	1.471 (3)	C16—H16C	0.9600
N1 ⁱ —Mn1—N1	180.0	N3—C7—H7	119.0
N1—Mn1—N2	93.63 (7)	C6—C7—H7	119.0
N1—Mn1—N2 ⁱ	86.37 (7)	C9—C8—N3	119.49 (19)
N1 ⁱ —Mn1—N2	86.37 (7)	C13—C8—N3	119.39 (19)
N1 ⁱ —Mn1—N2 ⁱ	93.63 (7)	C13—C8—C9	121.1 (2)
N1—Mn1—N3 ⁱ	91.50 (7)	C8—C9—C14	122.8 (2)
N1—Mn1—N3	88.50 (7)	C10—C9—C8	118.0 (2)
N1 ⁱ —Mn1—N3	91.50 (7)	C10—C9—C14	119.2 (2)
N1 ⁱ —Mn1—N3 ⁱ	88.50 (7)	C9—C10—H10	118.8
N2—Mn1—N2 ⁱ	180.0	C11—C10—C9	122.4 (2)
N2 ⁱ —Mn1—N3 ⁱ	74.26 (6)	C11—C10—H10	118.8
N2 ⁱ —Mn1—N3	105.74 (6)	C10—C11—C15	120.3 (2)
N2—Mn1—N3	74.26 (6)	C12—C11—C10	117.7 (2)
N2—Mn1—N3 ⁱ	105.74 (6)	C12—C11—C15	122.0 (2)
N3 ⁱ —Mn1—N3	180.00 (7)	C11—C12—H12	118.6
C1—N1—Mn1	164.27 (19)	C11—C12—C13	122.8 (2)
C2—N2—Mn1	129.08 (15)	C13—C12—H12	118.6
C2—N2—C6	117.55 (19)	C8—C13—C16	121.9 (2)
C6—N2—Mn1	113.30 (14)	C12—C13—C8	118.0 (2)
C7—N3—Mn1	112.59 (15)	C12—C13—C16	120.1 (2)
C7—N3—C8	116.82 (19)	C9—C14—H14A	109.5
C8—N3—Mn1	129.81 (13)	C9—C14—H14B	109.5
N1—C1—S1	179.4 (2)	C9—C14—H14C	109.5
N2—C2—H2	118.5	H14A—C14—H14B	109.5
N2—C2—C3	123.1 (2)	H14A—C14—H14C	109.5
C3—C2—H2	118.5	H14B—C14—H14C	109.5
C2—C3—H3	120.5	C11—C15—H15A	109.5
C4—C3—C2	119.0 (2)	C11—C15—H15B	109.5
C4—C3—H3	120.5	C11—C15—H15C	109.5
C3—C4—H4	120.3	H15A—C15—H15B	109.5
C3—C4—C5	119.4 (2)	H15A—C15—H15C	109.5
C5—C4—H4	120.3	H15B—C15—H15C	109.5
C4—C5—H5	120.8	C13—C16—H16A	109.5
C4—C5—C6	118.4 (2)	C13—C16—H16B	109.5
C6—C5—H5	120.8	C13—C16—H16C	109.5
N2—C6—C5	122.6 (2)	H16A—C16—H16B	109.5
N2—C6—C7	117.45 (19)	H16A—C16—H16C	109.5
C5—C6—C7	119.9 (2)	H16B—C16—H16C	109.5
N3—C7—C6	122.1 (2)		

Mn1—N2—C2—C3	-177.25 (17)	C5—C6—C7—N3	-175.9 (2)
Mn1—N2—C6—C5	176.51 (18)	C6—N2—C2—C3	-0.8 (3)
Mn1—N2—C6—C7	-6.3 (2)	C7—N3—C8—C9	66.4 (3)
Mn1—N3—C7—C6	-3.2 (3)	C7—N3—C8—C13	-115.6 (2)
Mn1—N3—C8—C9	-102.6 (2)	C8—N3—C7—C6	-174.13 (19)
Mn1—N3—C8—C13	75.4 (2)	C8—C9—C10—C11	0.9 (4)
N2—C2—C3—C4	1.6 (4)	C9—C8—C13—C12	-1.9 (3)
N2—C6—C7—N3	6.8 (3)	C9—C8—C13—C16	-179.9 (2)
N3—C8—C9—C10	179.25 (19)	C9—C10—C11—C12	-2.3 (4)
N3—C8—C9—C14	-0.3 (3)	C9—C10—C11—C15	175.6 (2)
N3—C8—C13—C12	-179.89 (19)	C10—C11—C12—C13	1.7 (4)
N3—C8—C13—C16	2.1 (3)	C11—C12—C13—C8	0.4 (3)
C2—N2—C6—C5	-0.5 (3)	C11—C12—C13—C16	178.4 (2)
C2—N2—C6—C7	176.70 (19)	C13—C8—C9—C10	1.2 (3)
C2—C3—C4—C5	-1.0 (4)	C13—C8—C9—C14	-178.3 (2)
C3—C4—C5—C6	-0.1 (4)	C14—C9—C10—C11	-179.5 (2)
C4—C5—C6—N2	1.0 (4)	C15—C11—C12—C13	-176.3 (2)
C4—C5—C6—C7	-176.2 (2)		

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Hydrogen-bond geometry (\AA , $^\circ$)

Cg1 is the mid-point of the C1=N1 group. Cg2 and Cg3 are the centroids of the N2/C2—C6 and C8—C13 rings.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C3—H3 \cdots S1 ⁱⁱ	0.93	3.16	3.812 (3)	129
C4—H4 \cdots Cg1 ⁱⁱ	0.93	2.89	3.561 (3)	129
C5—H5 \cdots S1 ⁱⁱⁱ	0.93	3.00	3.785 (3)	143
C7—H7 \cdots S1 ⁱⁱⁱ	0.93	3.07	3.871 (2)	146
C14—H14A \cdots Cg1 ⁱⁱⁱ	0.96	2.89	3.779 (3)	153
C14—H14B \cdots Cg2 ⁱⁱⁱ	0.96	2.68	3.556 (3)	152
C16—H16C \cdots Cg3 ^{iv}	0.96	3.14	3.711 (3)	145

Symmetry codes: (ii) $x, y+1, z$; (iii) $-x, -y+1, -z+1$; (iv) $-x+1, -y+1, -z+2$.

trans-Bis(thiocyanato- κN)bis[2,4,6-trimethyl-*N*-[(pyridin-2-yl)methylidene]aniline- $\kappa^2 N, N'$]nickel(II) (2)

Crystal data

$[\text{Ni}(\text{NCS})_2(\text{C}_{15}\text{H}_{16}\text{N}_2)_2]$

$M_r = 623.46$

Monoclinic, $P2_1/n$

$a = 9.6156$ (5) \AA

$b = 12.6786$ (7) \AA

$c = 12.9870$ (7) \AA

$\beta = 101.250$ (2) $^\circ$

$V = 1552.85$ (14) \AA^3

$Z = 2$

$F(000) = 652$

$D_x = 1.333$ Mg m^{-3}

Mo $K\alpha$ radiation, $\lambda = 0.71073$ \AA

Cell parameters from 9899 reflections

$\theta = 2.9\text{--}26.0^\circ$

$\mu = 0.79$ mm^{-1}

$T = 296$ K

Block, yellow

$0.34 \times 0.3 \times 0.3$ mm

Data collection

BRUKER D8 QUEST CMOS PHOTON II
diffractometer

Radiation source: sealed x-ray tube

Graphite monochromator

Detector resolution: 7.39 pixels mm⁻¹

φ and ω scans

Absorption correction: multi-scan
(SADABS; Krause *et al.*, 2015)

$T_{\min} = 0.607$, $T_{\max} = 0.745$

16977 measured reflections

3037 independent reflections

2486 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.032$

$\theta_{\max} = 26.1^\circ$, $\theta_{\min} = 2.9^\circ$

$h = -11 \rightarrow 11$

$k = -15 \rightarrow 15$

$l = -16 \rightarrow 15$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.053$

$wR(F^2) = 0.104$

$S = 1.21$

3037 reflections

190 parameters

0 restraints

Primary atom site location: dual

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + 2.7087P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.70 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.46 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ni1	0.500000	0.500000	0.500000	0.03174 (15)
S1	0.30833 (12)	0.80667 (8)	0.64005 (9)	0.0656 (3)
N1	0.4244 (3)	0.6312 (2)	0.5593 (2)	0.0407 (6)
N2	0.7069 (3)	0.5629 (2)	0.5334 (2)	0.0376 (6)
N3	0.5103 (3)	0.58125 (19)	0.35336 (19)	0.0351 (6)
C1	0.3753 (3)	0.7033 (3)	0.5927 (2)	0.0380 (7)
C2	0.8053 (4)	0.5554 (3)	0.6204 (3)	0.0533 (9)
H2	0.783080	0.519973	0.677802	0.064*
C3	0.9390 (4)	0.5978 (4)	0.6293 (3)	0.0729 (13)
H3	1.005516	0.590034	0.691205	0.087*
C4	0.9733 (4)	0.6514 (4)	0.5467 (4)	0.0819 (15)
H4	1.062568	0.681377	0.551611	0.098*
C5	0.8729 (4)	0.6600 (4)	0.4559 (3)	0.0678 (12)
H5	0.893397	0.695433	0.398017	0.081*
C6	0.7414 (3)	0.6153 (3)	0.4521 (3)	0.0437 (8)
C7	0.6315 (3)	0.6226 (3)	0.3574 (3)	0.0444 (8)
H7	0.650545	0.658144	0.299091	0.053*
C8	0.4138 (3)	0.5878 (2)	0.2529 (2)	0.0372 (7)
C9	0.3021 (4)	0.6589 (3)	0.2392 (3)	0.0462 (8)
C10	0.2091 (4)	0.6604 (3)	0.1422 (3)	0.0545 (9)

H10	0.134814	0.708629	0.131543	0.065*
C11	0.2232 (4)	0.5933 (3)	0.0619 (3)	0.0517 (9)
C12	0.3352 (4)	0.5232 (3)	0.0780 (3)	0.0538 (9)
H12	0.345521	0.477030	0.024406	0.065*
C13	0.4330 (4)	0.5197 (3)	0.1723 (3)	0.0451 (8)
C14	0.2780 (5)	0.7328 (4)	0.3238 (3)	0.0732 (13)
H14A	0.250055	0.693336	0.379517	0.110*
H14B	0.204558	0.781995	0.295563	0.110*
H14C	0.364035	0.770498	0.350751	0.110*
C15	0.1202 (5)	0.5975 (4)	−0.0417 (3)	0.0734 (12)
H15A	0.029627	0.621583	−0.030483	0.110*
H15B	0.110203	0.528411	−0.072451	0.110*
H15C	0.155037	0.645291	−0.088141	0.110*
C16	0.5547 (5)	0.4432 (3)	0.1826 (3)	0.0675 (12)
H16A	0.642709	0.480996	0.199615	0.101*
H16B	0.550087	0.406302	0.117462	0.101*
H16C	0.548991	0.393416	0.237354	0.101*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0322 (3)	0.0306 (3)	0.0340 (3)	−0.0017 (2)	0.0105 (2)	−0.0011 (2)
S1	0.0730 (7)	0.0543 (6)	0.0761 (7)	0.0125 (5)	0.0307 (6)	−0.0150 (5)
N1	0.0474 (15)	0.0369 (15)	0.0401 (15)	0.0012 (12)	0.0139 (12)	−0.0028 (12)
N2	0.0351 (13)	0.0347 (14)	0.0434 (15)	−0.0050 (11)	0.0087 (11)	−0.0019 (11)
N3	0.0400 (14)	0.0316 (13)	0.0355 (13)	0.0054 (11)	0.0117 (11)	0.0039 (11)
C1	0.0377 (16)	0.0437 (19)	0.0340 (16)	−0.0035 (14)	0.0105 (13)	0.0018 (14)
C2	0.048 (2)	0.062 (2)	0.047 (2)	−0.0088 (18)	0.0038 (16)	−0.0006 (18)
C3	0.046 (2)	0.102 (4)	0.064 (3)	−0.016 (2)	−0.0051 (19)	−0.004 (3)
C4	0.043 (2)	0.112 (4)	0.089 (3)	−0.030 (2)	0.008 (2)	0.005 (3)
C5	0.050 (2)	0.083 (3)	0.073 (3)	−0.023 (2)	0.017 (2)	0.011 (2)
C6	0.0392 (17)	0.0463 (19)	0.0479 (19)	−0.0060 (15)	0.0142 (15)	0.0020 (15)
C7	0.0480 (19)	0.0442 (19)	0.0441 (18)	−0.0028 (15)	0.0169 (15)	0.0078 (15)
C8	0.0398 (16)	0.0388 (17)	0.0338 (16)	0.0008 (13)	0.0093 (13)	0.0053 (13)
C9	0.0468 (19)	0.047 (2)	0.0453 (19)	0.0090 (16)	0.0105 (15)	0.0071 (16)
C10	0.049 (2)	0.057 (2)	0.057 (2)	0.0144 (17)	0.0078 (17)	0.0106 (18)
C11	0.056 (2)	0.050 (2)	0.046 (2)	−0.0018 (17)	0.0022 (16)	0.0097 (17)
C12	0.072 (2)	0.050 (2)	0.0376 (18)	0.0048 (18)	0.0062 (17)	0.0020 (15)
C13	0.056 (2)	0.0425 (19)	0.0383 (17)	0.0090 (15)	0.0121 (15)	0.0079 (14)
C14	0.085 (3)	0.073 (3)	0.059 (2)	0.033 (2)	0.008 (2)	−0.006 (2)
C15	0.073 (3)	0.078 (3)	0.061 (3)	0.002 (2)	−0.008 (2)	0.007 (2)
C16	0.089 (3)	0.072 (3)	0.043 (2)	0.036 (2)	0.016 (2)	0.0029 (19)

Geometric parameters (Å, °)

Ni1—N1	2.027 (3)	C7—H7	0.9300
Ni1—N1 ⁱ	2.027 (3)	C8—C9	1.387 (4)
Ni1—N2 ⁱ	2.108 (2)	C8—C13	1.398 (4)

Ni1—N2	2.108 (2)	C9—C10	1.395 (5)
Ni1—N3	2.184 (2)	C9—C14	1.496 (5)
Ni1—N3 ⁱ	2.184 (2)	C10—H10	0.9300
S1—C1	1.632 (3)	C10—C11	1.373 (5)
N1—C1	1.152 (4)	C11—C12	1.380 (5)
N2—C2	1.329 (4)	C11—C15	1.508 (5)
N2—C6	1.343 (4)	C12—H12	0.9300
N3—C7	1.269 (4)	C12—C13	1.391 (5)
N3—C8	1.448 (4)	C13—C16	1.506 (5)
C2—H2	0.9300	C14—H14A	0.9600
C2—C3	1.378 (5)	C14—H14B	0.9600
C3—H3	0.9300	C14—H14C	0.9600
C3—C4	1.363 (6)	C15—H15A	0.9600
C4—H4	0.9300	C15—H15B	0.9600
C4—C5	1.374 (6)	C15—H15C	0.9600
C5—H5	0.9300	C16—H16A	0.9600
C5—C6	1.377 (5)	C16—H16B	0.9600
C6—C7	1.459 (5)	C16—H16C	0.9600
N1—Ni1—N1 ⁱ	180.00 (14)	N3—C7—H7	119.4
N1 ⁱ —Ni1—N2	89.71 (10)	C6—C7—H7	119.4
N1 ⁱ —Ni1—N2 ⁱ	90.29 (10)	C9—C8—N3	119.8 (3)
N1—Ni1—N2	90.29 (10)	C9—C8—C13	121.2 (3)
N1—Ni1—N2 ⁱ	89.71 (10)	C13—C8—N3	118.9 (3)
N1 ⁱ —Ni1—N3 ⁱ	91.41 (10)	C8—C9—C10	117.9 (3)
N1 ⁱ —Ni1—N3	88.59 (10)	C8—C9—C14	122.6 (3)
N1—Ni1—N3	91.41 (10)	C10—C9—C14	119.4 (3)
N1—Ni1—N3 ⁱ	88.59 (10)	C9—C10—H10	118.8
N2—Ni1—N2 ⁱ	180.0	C11—C10—C9	122.5 (3)
N2 ⁱ —Ni1—N3 ⁱ	78.43 (10)	C11—C10—H10	118.8
N2 ⁱ —Ni1—N3	101.57 (10)	C10—C11—C12	118.2 (3)
N2—Ni1—N3	78.43 (10)	C10—C11—C15	120.7 (4)
N2—Ni1—N3 ⁱ	101.57 (10)	C12—C11—C15	121.1 (4)
N3 ⁱ —Ni1—N3	180.00 (13)	C11—C12—H12	119.1
C1—N1—Ni1	176.7 (3)	C11—C12—C13	121.9 (3)
C2—N2—Ni1	129.4 (2)	C13—C12—H12	119.1
C2—N2—C6	117.4 (3)	C8—C13—C16	123.1 (3)
C6—N2—Ni1	113.2 (2)	C12—C13—C8	118.3 (3)
C7—N3—Ni1	110.9 (2)	C12—C13—C16	118.7 (3)
C7—N3—C8	115.8 (3)	C9—C14—H14A	109.5
C8—N3—Ni1	133.02 (19)	C9—C14—H14B	109.5
N1—C1—S1	179.0 (3)	C9—C14—H14C	109.5
N2—C2—H2	118.6	H14A—C14—H14B	109.5
N2—C2—C3	122.8 (4)	H14A—C14—H14C	109.5
C3—C2—H2	118.6	H14B—C14—H14C	109.5
C2—C3—H3	120.2	C11—C15—H15A	109.5
C4—C3—C2	119.6 (4)	C11—C15—H15B	109.5
C4—C3—H3	120.2	C11—C15—H15C	109.5

C3—C4—H4	120.7	H15A—C15—H15B	109.5
C3—C4—C5	118.5 (4)	H15A—C15—H15C	109.5
C5—C4—H4	120.7	H15B—C15—H15C	109.5
C4—C5—H5	120.5	C13—C16—H16A	109.5
C4—C5—C6	119.0 (4)	C13—C16—H16B	109.5
C6—C5—H5	120.5	C13—C16—H16C	109.5
N2—C6—C5	122.7 (3)	H16A—C16—H16B	109.5
N2—C6—C7	116.4 (3)	H16A—C16—H16C	109.5
C5—C6—C7	120.9 (3)	H16B—C16—H16C	109.5
N3—C7—C6	121.1 (3)		
Ni1—N2—C2—C3	177.4 (3)	C5—C6—C7—N3	179.8 (4)
Ni1—N2—C6—C5	-178.0 (3)	C6—N2—C2—C3	-0.6 (6)
Ni1—N2—C6—C7	1.7 (4)	C7—N3—C8—C9	-105.0 (3)
Ni1—N3—C7—C6	-1.6 (4)	C7—N3—C8—C13	76.9 (4)
Ni1—N3—C8—C9	82.2 (4)	C8—N3—C7—C6	-176.0 (3)
Ni1—N3—C8—C13	-96.0 (3)	C8—C9—C10—C11	1.2 (5)
N2—C2—C3—C4	0.9 (7)	C9—C8—C13—C12	-1.4 (5)
N2—C6—C7—N3	0.0 (5)	C9—C8—C13—C16	178.4 (3)
N3—C8—C9—C10	-178.1 (3)	C9—C10—C11—C12	-1.0 (6)
N3—C8—C9—C14	1.7 (5)	C9—C10—C11—C15	179.9 (4)
N3—C8—C13—C12	176.8 (3)	C10—C11—C12—C13	-0.4 (6)
N3—C8—C13—C16	-3.5 (5)	C11—C12—C13—C8	1.6 (5)
C2—N2—C6—C5	0.3 (5)	C11—C12—C13—C16	-178.2 (4)
C2—N2—C6—C7	-179.9 (3)	C13—C8—C9—C10	0.0 (5)
C2—C3—C4—C5	-0.9 (8)	C13—C8—C9—C14	179.8 (4)
C3—C4—C5—C6	0.6 (8)	C14—C9—C10—C11	-178.6 (4)
C4—C5—C6—N2	-0.3 (7)	C15—C11—C12—C13	178.6 (4)
C4—C5—C6—C7	179.9 (4)		

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Hydrogen-bond geometry (\AA , $^\circ$)

Cg1 is the mid-point of the C1=N1 group.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C4—H4 \cdots S1 ⁱⁱ	0.93	2.89	3.769 (4)	158
C7—H7 \cdots S1 ⁱⁱⁱ	0.93	2.83	3.680 (3)	153
C10—H10 \cdots S1 ^{iv}	0.93	3.17	3.871 (4)	134
C10—H10 \cdots Cg1 ^{iv}	0.93	2.73	3.655 (4)	171

Symmetry codes: (ii) $x+1, y, z$; (iii) $x+1/2, -y+3/2, z-1/2$; (iv) $x-1/2, -y+3/2, z-1/2$.