Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis(thiocyanato-κN)tetrakis(1-vinyl-1*H*-imidazole-κN^3)nickel(II)

Su-Juan Pang,[a,c]* Juan Su[b] and Qiang Lin[c]

[a]Science and Engineering College, Hainan University, Haikou 570228, People's Republic of China, [b]Enrolment and Vocation Office, Qingdao Technical College, Qingdao 266555, People's Republic of China, and [c]Key Laboratory of Tropical Biological Resources of the Ministry of Education, Hainan University, Haikou 570228, People's Republic of China
Correspondence e-mail: husjpang@163.com

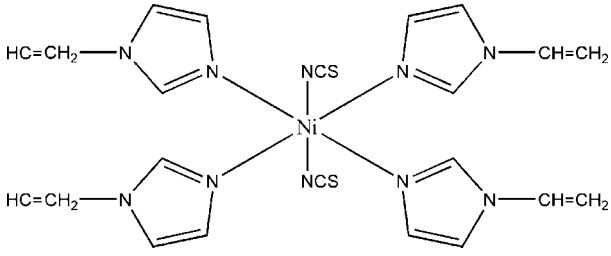
Received 10 August 2007; accepted 11 August 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.014 Å; R factor = 0.052; wR factor = 0.198; data-to-parameter ratio = 17.1.

The title compound, $[Ni(NCS)_2(C_5H_6N_2)_4]$, crystallizes with two independent half-molecules in the asymmetric unit; each Ni atom lies on a centre of symmetry. In both independent molecules, each Ni^{II} ion displays a compressed octahedral coordination geometry, with six N atoms from two thiocyanate anions and four 1-vinylimidazole ligands building the NiN_6 chromophore. In the crystal structure, π–π stacking interactions [centroid-to-centroid distance = 4.685 (3) Å] link the two independent molecules into a one-dimensional chain running along the a axis. Intermolecular C—H···S hydrogen bonds further stabilize the crystal structure.

Related literature

For related literature, see: Liu *et al.* (2005, 2006).



Experimental

Crystal data

$[Ni(NCS)_2(C_5H_6N_2)_4]$
M_r = 551.34
Triclinic, $P\overline{1}$
a = 9.6400 (19) Å
b = 10.242 (2) Å
c = 14.705 (3) Å
α = 109.46 (3)°
β = 90.16 (3)°
γ = 100.16 (3)°
V = 1344.5 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.91 mm^{-1}
T = 293 (2) K
0.30 × 0.30 × 0.20 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.773, T_{max} = 0.839
5593 measured reflections
5257 independent reflections
3080 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.198
S = 1.01
5257 reflections
307 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.66 e Å^{-3}
$\Delta\rho_{min}$ = −1.65 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7A···S1^{i}	0.93	2.86	3.638 (8)	142
C10—H10A···S1^{i}	0.93	2.79	3.601 (8)	146
C16—H16A···S1^{ii}	0.93	2.85	3.717 (18)	155

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and local programs.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2278).

References

Bruker (2001). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Liu, F.-Q., Chen, H.-N., Li, R.-X., Liu, G.-Y. & Li, W.-H. (2006). *Acta Cryst.* E**62**, m2457–m2458.
Liu, F.-Q., Jian, F.-F., Lu, L.-D., Yang, X.-J., Wang, X. & Xiao, H.-L. (2005). *Acta Cryst.* E**61**, m425–m426.
Sheldrick, G. M. (2001). *SHELXTL*. Version 5.0. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2004). *SADABS*. University of Göttingen, Germany.

 © 2007 International Union of Crystallography

supplementary materials

Acta Cryst. (2007). E**63**, m2369 [**doi:10.1107/S1600536807039888**]

Bis(thiocyanato-κN)tetrakis(1-vinyl-1*H*-imidazole-κN^3)nickel(II)

S.-J. Pang, J. Su and Q. Lin

Comment

The title compound, (I), crystallizes with two independent molecules in the asymmetric unit (Fig. 1). In the two independent molecules, each Ni^{II} ion, which are located on crystallographic centres of symmetry, displays a compressed octahedral coordination geometry, with six N atoms from two thiocyanate anions and four 1-vinylimidazole ligands building the NiN_6 chromophore. The equatorial planes in the two independent molecules are formed by four Ni—*N*(1-vinylimadazole) bonds with lengths ranging from 2.106 (5) to 2.118 (6) Å, and the axial positions are occupied by two N-bonded NCS groups [Ni—N(NCS) = 2.067 (6) and 2.065 (5) Å]. These values agree well with those observed in $[Ni(NCS)_2(1\text{-methylimidazole})_4]$ (Liu *et al.*, 2005) and $[Ni(NCS)_2(1\text{-ethylimidazole})_4]$ (Liu *et al.*, 2006). In the crystal, the distance of 4.685 (3)Å of *Cg*1···*Cg*1 [*Cg*1 is centroids of N9–N10/C18–C20; symmetry code: 1-*X*,-Y,1-*Z*] shows a presence of π···π stacking interactions which link the two independent molecules into 1-D chain running along the *a* axis. Intermolecular C—H···S hydrogen bonds further stabilize the crystal structure.

Experimental

The title compound was prepared by the reaction of 1-vinylimidazole (1.88 g, 20 mmol) with $NiCl_2{\cdot}6H_2O$(1.19 g, 5 mmol) and potassium thiocyanate (0.98 g, 10 mmol) by means of hydrothermal synthesis in a stainless-steel reactor with Teflon liner at 383 K for 24 h. Single crystals suitable for X-ray measurements were obtained by recrystallization from methanol at room temperature.

Refinement

H atoms were positioned geometrically and allowed to ride on their attached atoms, with C—H distances = 0.93–0.96 Å, and with U_{iso}(H) = 1.2–1.5U_{eq}(C).

Figures

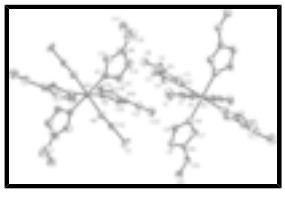


Fig. 1. The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

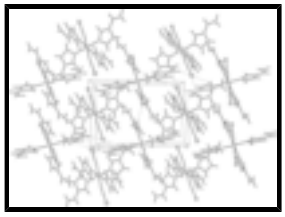


Fig. 2. The packing of (I), viewed down the *b* axis.

Bis(thiocyanato-κ*N*)tetrakis(1-vinyl-1*H*-imidazole-κN^3)nickel(II)

Crystal data

$[Ni(NCS)_2(C_5H_6N_2)_4]$	$Z = 2$
$M_r = 551.34$	$F_{000} = 572$
Triclinic, $P\overline{1}$	$D_x = 1.362$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.6400$ (19) Å	Cell parameters from 3253 reflections
$b = 10.242$ (2) Å	$\theta = 4$–14º
$c = 14.705$ (3) Å	$\mu = 0.91$ mm^{-1}
$\alpha = 109.46$ (3)º	$T = 293$ (2) K
$\beta = 90.16$ (3)º	Block, blue
$\gamma = 100.16$ (3)º	0.30 × 0.30 × 0.20 mm
$V = 1344.5$ (6) Å^3	

Data collection

Bruker SMART 1K CCD area-detector diffractometer	5257 independent reflections
Radiation source: fine-focus sealed tube	3080 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.034$
$T = 293$(2) K	$\theta_{max} = 26.0$º
thin–slice ω scans	$\theta_{min} = 1.5$º
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)	$h = 0 \rightarrow 11$
$T_{min} = 0.773$, $T_{max} = 0.839$	$k = -12 \rightarrow 12$
5593 measured reflections	$l = -18 \rightarrow 18$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.052$	H-atom parameters constrained
$wR(F^2) = 0.198$	$w = 1/[\sigma^2(F_o^2) + (0.1152P)^2 + 2.8055P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} = 0.032$
5257 reflections	$\Delta\rho_{max} = 0.66$ e Å^{-3}

307 parameters	$\Delta\rho_{min} = -1.65$ e Å^{-3}
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Ni1	0.5000	0.0000	0.0000	0.0496 (4)
S1	0.0867 (3)	0.2078 (3)	0.07754 (18)	0.0870 (8)
N1	0.3250 (7)	0.0951 (7)	0.0234 (4)	0.0646 (17)
N3	0.3709 (9)	−0.3102 (8)	0.1314 (6)	0.080 (2)
N2	0.4058 (6)	−0.1414 (7)	0.0687 (4)	0.0597 (16)
N5	0.7598 (6)	0.2755 (6)	0.2474 (4)	0.0493 (13)
N4	0.5948 (6)	0.1415 (6)	0.1351 (4)	0.0530 (14)
C6	0.3214 (10)	−0.4777 (10)	0.2129 (7)	0.085
H6A	0.2422	−0.4401	0.2361	0.102*
H6B	0.3430	−0.5524	0.2293	0.102*
C5	0.4024 (15)	−0.4254 (13)	0.1574 (9)	0.122 (4)
H5A	0.4815	−0.4634	0.1345	0.147*
C3	0.2604 (12)	−0.2492 (12)	0.1510 (8)	0.099 (3)
H3A	0.1837	−0.2739	0.1841	0.118*
C4	0.2797 (9)	−0.1443 (11)	0.1141 (7)	0.086 (3)
H4A	0.2178	−0.0827	0.1182	0.104*
C2	0.4563 (10)	−0.2409 (9)	0.0822 (7)	0.076 (2)
H2A	0.5425	−0.2637	0.0607	0.091*
C11	0.9296 (9)	0.4409 (8)	0.3719 (6)	0.068 (2)
H11A	0.8578	0.4784	0.4077	0.082*
H11B	1.0235	0.4767	0.3948	0.082*
C10	0.8991 (8)	0.3395 (8)	0.2904 (5)	0.0562 (18)
H10A	0.9740	0.3051	0.2569	0.067*
C8	0.6330 (8)	0.3001 (8)	0.2836 (5)	0.0569 (18)
H8A	0.6186	0.3615	0.3441	0.068*
C9	0.5329 (8)	0.2177 (8)	0.2143 (5)	0.0584 (19)
H9A	0.4361	0.2131	0.2194	0.070*
C7	0.7300 (8)	0.1789 (8)	0.1588 (5)	0.0566 (18)
H7A	0.7984	0.1424	0.1185	0.068*

C1	0.2269 (7)	0.1420 (8)	0.0464 (5)	0.0520 (17)
Ni2	0.0000	0.0000	0.5000	0.0402 (3)
S2	0.3353 (2)	0.3734 (2)	0.4538 (2)	0.0853 (8)
N6	0.1136 (6)	0.1787 (6)	0.4808 (5)	0.0547 (15)
N8	−0.1142 (8)	−0.2379 (10)	0.2048 (5)	0.086 (3)
N7	−0.0582 (6)	−0.0859 (6)	0.3503 (4)	0.0514 (14)
N10	0.3853 (6)	−0.1437 (6)	0.4179 (4)	0.0526 (14)
N9	0.1789 (5)	−0.0955 (5)	0.4706 (4)	0.0459 (13)
C17	−0.1907 (10)	−0.4674 (10)	0.1355 (8)	0.087
H17A	−0.1961	−0.4693	0.1982	0.104*
H17B	−0.2163	−0.5504	0.0831	0.104*
C16	−0.1493 (15)	−0.3543 (14)	0.1217 (11)	0.145 (5)
H16A	−0.1424	−0.3481	0.0601	0.174*
C14	−0.0759 (10)	−0.1120 (11)	0.1937 (7)	0.079 (3)
H14A	−0.0746	−0.0929	0.1361	0.095*
C15	−0.0403 (8)	−0.0209 (9)	0.2817 (5)	0.065 (2)
H15A	−0.0074	0.0751	0.2956	0.077*
C13	−0.1039 (9)	−0.2177 (9)	0.3013 (7)	0.074 (2)
H13A	−0.1265	−0.2886	0.3281	0.089*
C22	0.5619 (9)	−0.0592 (11)	0.3267 (7)	0.087 (3)
H22A	0.5062	−0.0005	0.3147	0.104*
H22B	0.6506	−0.0615	0.3022	0.104*
C21	0.5170 (8)	−0.1359 (9)	0.3762 (6)	0.067 (2)
H21A	0.5765	−0.1928	0.3862	0.080*
C19	0.3321 (9)	−0.2359 (8)	0.4646 (6)	0.065 (2)
H19A	0.3747	−0.3059	0.4733	0.079*
C20	0.2070 (8)	−0.2054 (8)	0.4953 (6)	0.0607 (19)
H20A	0.1478	−0.2527	0.5287	0.073*
C18	0.2891 (7)	−0.0618 (7)	0.4241 (5)	0.0493 (16)
H18A	0.2988	0.0108	0.3985	0.059*
C12	0.2049 (7)	0.2587 (6)	0.4678 (5)	0.0449 (15)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0353 (7)	0.0620 (8)	0.0486 (8)	0.0122 (6)	0.0028 (5)	0.0136 (6)
S1	0.0682 (14)	0.123 (2)	0.0795 (16)	0.0500 (14)	0.0290 (12)	0.0312 (15)
N1	0.054 (4)	0.076 (5)	0.057 (4)	0.023 (3)	0.006 (3)	0.009 (3)
N3	0.090 (6)	0.069 (5)	0.082 (5)	−0.001 (4)	−0.009 (4)	0.034 (4)
N2	0.052 (4)	0.067 (4)	0.055 (4)	0.002 (3)	−0.005 (3)	0.019 (3)
N5	0.048 (3)	0.056 (3)	0.043 (3)	0.011 (3)	0.006 (3)	0.015 (3)
N4	0.045 (3)	0.062 (4)	0.047 (3)	0.010 (3)	0.003 (3)	0.011 (3)
C6	0.085	0.085	0.085	0.016	0.006	0.029
C5	0.046 (4)	0.065 (5)	0.039 (4)	0.011 (4)	0.001 (3)	0.010 (3)
C3	0.083 (7)	0.120 (9)	0.100 (8)	−0.003 (7)	0.003 (6)	0.058 (7)
C4	0.064 (6)	0.112 (8)	0.097 (7)	0.010 (5)	0.018 (5)	0.057 (6)
C2	0.069 (6)	0.072 (6)	0.086 (6)	0.010 (5)	−0.002 (5)	0.026 (5)
C11	0.072 (5)	0.063 (5)	0.061 (5)	0.006 (4)	−0.004 (4)	0.014 (4)

C10	0.055 (4)	0.058 (4)	0.048 (4)	0.005 (3)	0.003 (3)	0.011 (4)
C8	0.062 (5)	0.060 (4)	0.043 (4)	0.013 (4)	0.006 (3)	0.011 (3)
C9	0.052 (4)	0.075 (5)	0.050 (4)	0.020 (4)	0.006 (3)	0.020 (4)
C7	0.049 (4)	0.068 (5)	0.046 (4)	0.009 (3)	0.004 (3)	0.011 (4)
C1	0.046 (4)	0.065 (5)	0.039 (4)	0.011 (4)	0.001 (3)	0.010 (3)
Ni2	0.0363 (6)	0.0390 (6)	0.0454 (7)	−0.0030 (5)	−0.0010 (5)	0.0197 (5)
S2	0.0629 (13)	0.0617 (13)	0.134 (2)	−0.0008 (10)	0.0420 (14)	0.0422 (14)
N6	0.052 (3)	0.047 (3)	0.068 (4)	−0.002 (3)	0.004 (3)	0.029 (3)
N8	0.073 (4)	0.103 (5)	0.054 (3)	0.022 (3)	−0.020 (3)	−0.012 (3)
N7	0.049 (3)	0.053 (4)	0.052 (3)	0.005 (3)	−0.004 (3)	0.019 (3)
N10	0.043 (3)	0.054 (3)	0.059 (4)	0.012 (3)	0.002 (3)	0.017 (3)
N9	0.042 (3)	0.046 (3)	0.053 (3)	0.004 (2)	−0.001 (3)	0.022 (3)
C17	0.087	0.087	0.087	0.016	0.006	0.029
C16	0.148 (3)	0.067 (4)	0.037 (3)	0.009 (3)	0.000 (2)	0.010 (3)
C14	0.072 (6)	0.101 (8)	0.068 (6)	0.021 (5)	0.000 (5)	0.032 (6)
C15	0.067 (5)	0.080 (5)	0.050 (5)	0.014 (4)	−0.001 (4)	0.025 (4)
C13	0.069 (5)	0.067 (5)	0.075 (6)	0.003 (4)	−0.017 (4)	0.016 (5)
C22	0.053 (5)	0.124 (8)	0.080 (6)	0.009 (5)	0.002 (4)	0.033 (6)
C21	0.052 (5)	0.076 (5)	0.071 (5)	0.013 (4)	0.010 (4)	0.020 (5)
C19	0.072 (5)	0.055 (4)	0.084 (6)	0.028 (4)	0.015 (4)	0.035 (4)
C20	0.067 (5)	0.052 (4)	0.073 (5)	0.011 (4)	0.013 (4)	0.034 (4)
C18	0.049 (4)	0.054 (4)	0.045 (4)	0.002 (3)	0.001 (3)	0.022 (3)
C12	0.049 (4)	0.039 (3)	0.050 (4)	0.011 (3)	0.011 (3)	0.017 (3)

Geometric parameters (Å, °)

Ni1—N1^{i}	2.067 (6)	Ni2—N6^{ii}	2.065 (5)
Ni1—N1	2.067 (6)	Ni2—N6	2.065 (5)
Ni1—N2	2.111 (6)	Ni2—N9	2.106 (5)
Ni1—N2^{i}	2.111 (6)	Ni2—N9^{ii}	2.106 (5)
Ni1—N4^{i}	2.118 (6)	Ni2—N7	2.113 (6)
Ni1—N4	2.118 (6)	Ni2—N7^{ii}	2.113 (6)
S1—C1	1.615 (7)	S2—C12	1.626 (7)
N1—C1	1.138 (9)	N6—C12	1.155 (8)
N3—C3	1.313 (13)	N8—C14	1.341 (12)
N3—C2	1.358 (11)	N8—C13	1.366 (11)
N3—C5	1.434 (14)	N8—C16	1.383 (15)
N2—C2	1.276 (10)	N7—C13	1.294 (10)
N2—C4	1.388 (10)	N7—C15	1.378 (9)
N5—C7	1.341 (9)	N10—C18	1.340 (9)
N5—C8	1.366 (9)	N10—C19	1.375 (9)
N5—C10	1.429 (9)	N10—C21	1.413 (9)
N4—C7	1.303 (8)	N9—C18	1.321 (8)
N4—C9	1.373 (9)	N9—C20	1.361 (8)
C6—C5	1.308 (14)	C17—C16	1.240 (19)
C6—H6A	0.9300	C17—H17A	0.9300
C6—H6B	0.9300	C17—H17B	0.9300
C5—H5A	0.9300	C16—H16A	0.9300

C3—C4	1.343 (13)	C14—C15	1.320 (11)
C3—H3A	0.9300	C14—H14A	0.9300
C4—H4A	0.9300	C15—H15A	0.9300
C2—H2A	0.9300	C13—H13A	0.9300
C11—C10	1.288 (10)	C22—C21	1.264 (12)
C11—H11A	0.9300	C22—H22A	0.9300
C11—H11B	0.9300	C22—H22B	0.9300
C10—H10A	0.9300	C21—H21A	0.9300
C8—C9	1.348 (10)	C19—C20	1.340 (10)
C8—H8A	0.9300	C19—H19A	0.9300
C9—H9A	0.9300	C20—H20A	0.9300
C7—H7A	0.9300	C18—H18A	0.9300
$N1^{i}$—Ni1—N1	180.0 (3)	$N6^{ii}$—Ni2—N6	180.00 (18)
$N1^{i}$—Ni1—N2	90.5 (3)	$N6^{ii}$—Ni2—N9	90.4 (2)
N1—Ni1—N2	89.5 (3)	N6—Ni2—N9	89.6 (2)
$N1^{i}$—Ni1—$N2^{i}$	89.5 (3)	$N6^{ii}$—Ni2—$N9^{ii}$	89.6 (2)
N1—Ni1—$N2^{i}$	90.5 (3)	N6—Ni2—$N9^{ii}$	90.4 (2)
N2—Ni1—$N2^{i}$	180.0 (3)	N9—Ni2—$N9^{ii}$	180.0 (3)
$N1^{i}$—Ni1—$N4^{i}$	89.7 (2)	$N6^{ii}$—Ni2—N7	90.2 (2)
N1—Ni1—$N4^{i}$	90.3 (2)	N6—Ni2—N7	89.8 (2)
N2—Ni1—$N4^{i}$	90.2 (2)	N9—Ni2—N7	87.7 (2)
$N2^{i}$—Ni1—$N4^{i}$	89.8 (2)	$N9^{ii}$—Ni2—N7	92.3 (2)
$N1^{i}$—Ni1—N4	90.3 (2)	$N6^{ii}$—Ni2—$N7^{ii}$	89.8 (2)
N1—Ni1—N4	89.7 (2)	N6—Ni2—$N7^{ii}$	90.2 (2)
N2—Ni1—N4	89.8 (2)	N9—Ni2—$N7^{ii}$	92.3 (2)
$N2^{i}$—Ni1—N4	90.2 (2)	$N9^{ii}$—Ni2—$N7^{ii}$	87.7 (2)
$N4^{i}$—Ni1—N4	180.0 (2)	N7—Ni2—$N7^{ii}$	180.000 (1)
C1—N1—Ni1	171.2 (7)	C12—N6—Ni2	162.1 (6)
C3—N3—C2	107.0 (8)	C14—N8—C13	107.9 (7)
C3—N3—C5	128.4 (10)	C14—N8—C16	117.1 (9)
C2—N3—C5	124.6 (10)	C13—N8—C16	134.9 (10)
C2—N2—C4	103.6 (8)	C13—N7—C15	104.7 (7)
C2—N2—Ni1	127.3 (6)	C13—N7—Ni2	126.1 (6)
C4—N2—Ni1	129.0 (6)	C15—N7—Ni2	128.7 (5)
C7—N5—C8	106.2 (6)	C18—N10—C19	105.5 (6)
C7—N5—C10	124.8 (6)	C18—N10—C21	128.4 (7)
C8—N5—C10	128.9 (6)	C19—N10—C21	126.1 (7)
C7—N4—C9	104.8 (6)	C18—N9—C20	104.6 (6)
C7—N4—Ni1	125.7 (5)	C18—N9—Ni2	127.7 (5)
C9—N4—Ni1	129.4 (5)	C20—N9—Ni2	127.8 (5)
C5—C6—H6A	120.0	C16—C17—H17A	120.0
C5—C6—H6B	120.0	C16—C17—H17B	120.0
H6A—C6—H6B	120.0	H17A—C17—H17B	120.0
C6—C5—N3	120.9 (13)	C17—C16—N8	114.9 (13)
C6—C5—H5A	119.6	C17—C16—H16A	122.5
N3—C5—H5A	119.6	N8—C16—H16A	122.6

N3—C3—C4	106.6 (9)	C15—C14—N8	105.5 (8)
N3—C3—H3A	126.7	C15—C14—H14A	127.2
C4—C3—H3A	126.7	N8—C14—H14A	127.2
C3—C4—N2	109.9 (9)	C14—C15—N7	111.5 (8)
C3—C4—H4A	125.0	C14—C15—H15A	124.3
N2—C4—H4A	125.0	N7—C15—H15A	124.3
N2—C2—N3	112.8 (9)	N7—C13—N8	110.4 (8)
N2—C2—H2A	123.6	N7—C13—H13A	124.8
N3—C2—H2A	123.6	N8—C13—H13A	124.8
C10—C11—H11A	120.0	C21—C22—H22A	120.0
C10—C11—H11B	120.0	C21—C22—H22B	120.0
H11A—C11—H11B	120.0	H22A—C22—H22B	120.0
C11—C10—N5	125.5 (7)	C22—C21—N10	126.4 (9)
C11—C10—H10A	117.3	C22—C21—H21A	116.8
N5—C10—H10A	117.3	N10—C21—H21A	116.8
C9—C8—N5	106.4 (6)	C20—C19—N10	106.9 (6)
C9—C8—H8A	126.8	C20—C19—H19A	126.6
N5—C8—H8A	126.8	N10—C19—H19A	126.6
C8—C9—N4	109.9 (7)	C19—C20—N9	110.4 (7)
C8—C9—H9A	125.0	C19—C20—H20A	124.8
N4—C9—H9A	125.0	N9—C20—H20A	124.8
N4—C7—N5	112.7 (6)	N9—C18—N10	112.6 (6)
N4—C7—H7A	123.7	N9—C18—H18A	123.7
N5—C7—H7A	123.7	N10—C18—H18A	123.7
N1—C1—S1	179.2 (7)	N6—C12—S2	177.9 (7)
$N1^{i}$—Ni1—N2—C2	−0.4 (7)	$N7^{ii}$—Ni2—N6—C12	87.5 (19)
N1—Ni1—N2—C2	179.6 (7)	$N6^{ii}$—Ni2—N7—C13	−19.3 (7)
$N4^{i}$—Ni1—N2—C2	89.2 (7)	N6—Ni2—N7—C13	160.7 (7)
N4—Ni1—N2—C2	−90.8 (7)	N9—Ni2—N7—C13	71.0 (7)
$N1^{i}$—Ni1—N2—C4	175.8 (7)	$N9^{ii}$—Ni2—N7—C13	−109.0 (7)
N1—Ni1—N2—C4	−4.2 (7)	$N6^{ii}$—Ni2—N7—C15	169.7 (6)
$N4^{i}$—Ni1—N2—C4	−94.6 (7)	N6—Ni2—N7—C15	−10.3 (6)
N4—Ni1—N2—C4	85.4 (7)	N9—Ni2—N7—C15	−100.0 (6)
$N1^{i}$—Ni1—N4—C7	25.0 (7)	$N9^{ii}$—Ni2—N7—C15	80.0 (6)
N1—Ni1—N4—C7	−155.0 (7)	$N6^{ii}$—Ni2—N9—C18	159.1 (6)
N2—Ni1—N4—C7	115.5 (6)	N6—Ni2—N9—C18	−20.9 (6)
$N2^{i}$—Ni1—N4—C7	−64.5 (6)	N7—Ni2—N9—C18	69.0 (6)
N1—Ni1—N4—C9	22.0 (7)	$N7^{ii}$—Ni2—N9—C18	−111.0 (6)
N2—Ni1—N4—C9	−67.5 (6)	$N6^{ii}$—Ni2—N9—C20	−21.0 (6)
$N2^{i}$—Ni1—N4—C9	112.5 (6)	N6—Ni2—N9—C20	159.0 (6)
C3—N3—C5—C6	−4.9 (18)	N7—Ni2—N9—C20	−111.1 (6)
C2—N3—C5—C6	173.2 (10)	$N7^{ii}$—Ni2—N9—C20	68.9 (6)
C2—N3—C3—C4	−0.1 (11)	C14—N8—C16—C17	−176.6 (11)
C5—N3—C3—C4	178.3 (10)	C13—N8—C16—C17	6(2)
N3—C3—C4—N2	0.8 (12)	C13—N8—C14—C15	1.6 (10)
C2—N2—C4—C3	−1.3 (11)	C16—N8—C14—C15	−176.5 (9)

Ni1—N2—C4—C3	−178.2 (6)	N8—C14—C15—N7	−1.4 (10)
C4—N2—C2—N3	1.2 (10)	C13—N7—C15—C14	0.6 (9)
Ni1—N2—C2—N3	178.2 (5)	Ni2—N7—C15—C14	173.1 (6)
C3—N3—C2—N2	−0.8 (11)	C15—N7—C13—N8	0.5 (9)
C5—N3—C2—N2	−179.3 (9)	Ni2—N7—C13—N8	−172.3 (5)
C7—N5—C10—C11	173.7 (8)	C14—N8—C13—N7	−1.4 (10)
C8—N5—C10—C11	−4.3 (12)	C16—N8—C13—N7	176.3 (11)
C7—N5—C8—C9	−0.6 (8)	C18—N10—C21—C22	−8.8 (14)
C10—N5—C8—C9	177.6 (7)	C19—N10—C21—C22	174.1 (9)
N5—C8—C9—N4	0.1 (9)	C18—N10—C19—C20	0.6 (8)
C7—N4—C9—C8	0.4 (9)	C21—N10—C19—C20	178.3 (7)
Ni1—N4—C9—C8	−177.1 (5)	N10—C19—C20—N9	−0.7 (9)
C9—N4—C7—N5	−0.9 (9)	C18—N9—C20—C19	0.4 (8)
Ni1—N4—C7—N5	176.7 (5)	Ni2—N9—C20—C19	−179.5 (5)
C8—N5—C7—N4	1.0 (9)	C20—N9—C18—N10	0.0 (8)
C10—N5—C7—N4	−177.4 (6)	Ni2—N9—C18—N10	179.9 (4)
N9—Ni2—N6—C12	−4.8 (19)	C19—N10—C18—N9	−0.4 (8)
$N9^{ii}$—Ni2—N6—C12	175.2 (19)	C21—N10—C18—N9	−178.0 (6)
N7—Ni2—N6—C12	−92.5 (19)		

Symmetry codes: (i) −*x*+1, −*y*, −*z*; (ii) −*x*, −*y*, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7A···$S1^{iii}$	0.93	2.86	3.638 (8)	142
C10—H10A···$S1^{iii}$	0.93	2.79	3.601 (8)	146
C16—H16A···$S1^{iv}$	0.93	2.85	3.717 (18)	155

Symmetry codes: (iii) *x*+1, *y*, *z*; (iv) −*x*, −*y*, −*z*.

Fig. 1

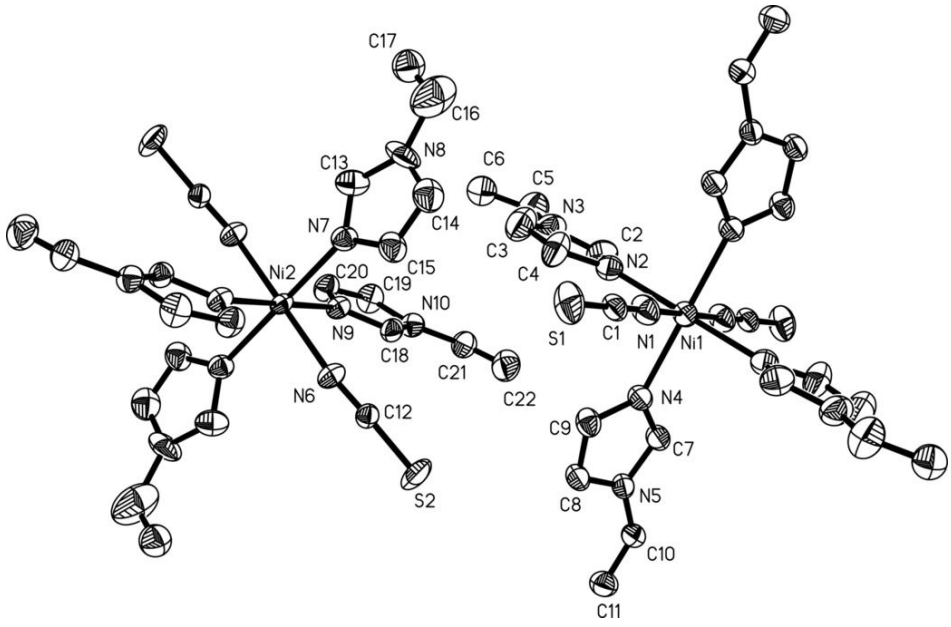

C17
C16
N8
C13
C6
C5
N3
N7
C14
C3
C2
Ni2
C20
C19
C15
C4
N2
N10
S1
C1
N1
Ni1
N9
C18
C21
C22
N6
C12
N4
C9
C7
S2
C8
N5
C10
C11

Fig. 2