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Bis(2,2′-diamino-4,4′-bi-1,3-thiazole-κ^2N,N')(2-nitrobenzoato-κ^2O,O')-nickel(II) 2-nitrobenzoate

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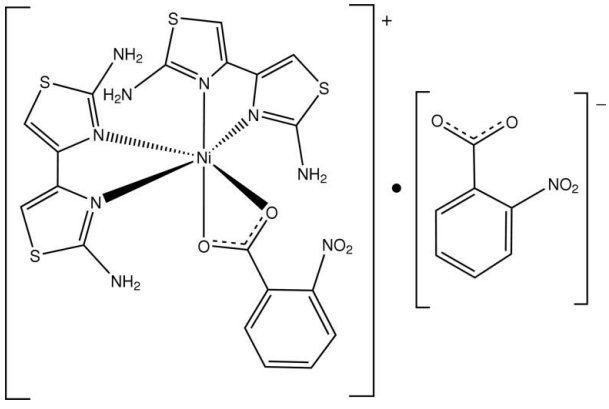
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.009 Å; R factor = 0.055; wR factor = 0.123; data-to-parameter ratio = 12.9.

The crystal structure of the title compound, $[Ni(C_7H_4NO_4)(C_6H_6N_4S_2)_2](C_7H_4NO_4)$, consists of Ni^{II} complex cations and 2-nitrobenzoate anions. The Ni^{II} ion assumes a distorted octahedral coordination geometry formed by one 2-nitrobenzoate anion and two diaminobithiazole ligands. N—H···O hydrogen bonding between cations and anions and between cations helps to stabilize the crystal structure.

Related literature

For general background, see Liu *et al.* (2001); Liu & Xu (2004). For related structures, see Liu & Xu (2003); Luo *et al.* (2004).



Experimental

Crystal data

$[Ni(C_7H_4NO_4)(C_6H_6N_4S_2)_2](C_7H_4NO_4)$
M_r = 787.47
Monoclinic, $P2_1/n$
a = 15.1514 (18) Å
b = 13.5905 (16) Å
c = 16.4702 (19) Å
β = 106.901 (2)°
V = 3245.0 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.92 mm^{-1}
T = 295 (2) K
0.20 × 0.17 × 0.14 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.812, T_{max} = 0.880
16530 measured reflections
5721 independent reflections
3217 reflections with $I > 2\sigma(I)$
R_{int} = 0.086

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.123
S = 1.00
5721 reflections
443 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ni—N11	2.073 (4)	Ni—N23	2.060 (4)
Ni—N13	2.078 (4)	Ni—O31	2.143 (3)
Ni—N21	2.073 (4)	Ni—O32	2.217 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
N12—H12A···O43^{i}	0.77	2.01	2.779 (6)	176
N12—H12B···O32	0.83	2.23	2.982 (6)	151
N12—H12B···O33	0.83	2.48	2.999 (6)	122
N14—H14A···O32^{ii}	0.95	2.06	2.953 (5)	156
N14—H14B···N21	0.89	2.32	3.114 (6)	149
N22—H22A···O31	0.87	2.20	2.886 (6)	136
N22—H22B···O44^{iii}	0.92	2.06	2.923 (6)	156
N24—H24A···N11	0.84	2.39	3.204 (5)	161
N24—H24B···O44^{iv}	0.84	2.13	2.810 (5)	137

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC & Rigaku, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2277).

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supplementary materials

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Bis(2,2'-diamino-4,4'-bi-1,3-thiazole-κ^2N,N')(2-nitrobenzoato-κ^2O,O')nickel(II) 2-nitrobenzoate

B.-X. Liu, G.-H. Chen, Y.-Y. Lin and Y.-P. Yu

Comment

Transition metal complexes of 2,2'-diamino-4,4'-bi-1,3-thiazole (DABT) have shown potential application in the field of soft magnetic material (Liu *et al.*, 2001). As part of serial structural investigation of metal complexes with DABT (Liu & Xu, 2004), the title Ni^{II} complex was recently prepared and its X-ray structure is presented here.

The molecular structure of the title compound is shown in Fig. 1. The Ni ion has a distorted octahedral coordinatation geometry formed by one 2-nitrobenzoate anion and two DABT ligands. Within the complex, two DABT moieties are approximately perpendicular to each other with a dihedral angle of 81.23 (7)°. This is comparable to 84.3 (4)° found in a Ni^{II} complex of DABT reported previously (Liu & Xu, 2003). Each DABT moiety is approximately coplanar coordinated to Ni atom, the dihedral angles between two thiazole rings being 6.2 (3) and 2.6 (2)°, respectively, which agree with 4.57 (7)° found in [Mn(DABT)(oxydiacetate)] (Luo *et al.*, 2004). The average Ni—N bond distance (Table 1) is shorter than the value of 2.113 (2) Å of average Ni—N bond distance found in reported Ni^{II} complex of DABT (Liu & Xu, 2003).

The extensive hydrogen bonding occurs in the crystal structure (Table 2). While 2-nitrobenzoate anion links with complex cation *via* N—H···O hydrogen bonding, the N—H···O hydrogen bonding is also observed between complex cations. They help to stabilize the crystal structure.

Experimental

An ethanol solution (20 ml) containing DABT (0.20 g, 1 mmol) and $NiCl_2·6H_2O$ (0.24 g, 1 mmol) was mixed with an aqueous solution (10 ml) of 2-nitrobenzoic acid (0.34 g, 2 mmol) and NaOH (0.08 g, 2 mmol). The mixture was refluxed for 6 h. After cooling to room temperature the solution was filtered. Single crystals of the title compound were obtained from the filtrate after 4 d.

Refinement

H atoms on carbon atoms were placed in calculated positions, with C—H distances = 0.93 Å (aromatic), and were included in the final cycles of refinement in riding mode with $U_{iso}(H) = 1.2U_{eq}(C)$. Amino H atoms were located in a difference Fourier map and included in the structure factor calculations with fixed positional and isotropic displacement parameters $U_{iso}(H) = 0.05$ Å^2.

Figures

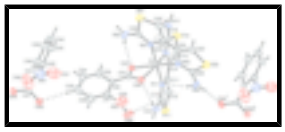


Fig. 1. The molecular structure of (I) with 30% probability displacement ellipsoids (arbitrary spheres for H atoms), dashed lines showing the hydrogen bonding [symmetry code: (i) *x*, *y*, *z* − 1].

Bis(2,2'-diamino-4,4'-bi-1,3-thiazole-κ^2*N*,*N*')(2-nitrobenzoato-\ κ^2*O*,*O*')nickel(II) 2-nitrobenzoate

Crystal data

$[Ni(C_7H_4NO_4)(C_6H_6N_4S_2)_2](C_7H_4NO_4)$	F_{000} = 1608
M_r = 787.47	D_x = 1.612 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 5670 reflections
a = 15.1514 (18) Å	θ = 2.0–25.0º
b = 13.5905 (16) Å	μ = 0.92 mm^{-1}
c = 16.4702 (19) Å	*T* = 295 (2) K
β = 106.901 (2)º	Prism, green
V = 3245.0 (7) Å^3	0.20 × 0.17 × 0.14 mm
Z = 4	

Data collection

Rigaku R-AXIS RAPID IP diffractometer	5721 independent reflections
Radiation source: fine-focus sealed tube	3217 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.086
Detector resolution: 10.0 pixels mm^{-1}	θ_{max} = 25.0º
T = 295(2) K	θ_{min} = 1.9º
ω scans	*h* = −16→18
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	*k* = −8→16
T_{min} = 0.812, T_{max} = 0.880	*l* = −18→19
16530 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.055	$w = 1/[\sigma^2(F_o^2) + (0.0399P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.123	$(\Delta/\sigma)_{max} < 0.001$
S = 1.00	$\Delta\rho_{max}$ = 0.42 e Å^{-3}
5721 reflections	$\Delta\rho_{min}$ = −0.37 e Å^{-3}

443 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0016 (3)

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}
Ni	0.63304 (4)	0.33644 (5)	0.24108 (4)	0.0312 (2)
N11	0.5040 (2)	0.2921 (3)	0.1665 (2)	0.0331 (10)
N12	0.4906 (3)	0.1244 (3)	0.1911 (3)	0.0561 (13)
H12A	0.4577	0.0832	0.1957	0.050*
H12B	0.5402	0.1254	0.2291	0.050*
N13	0.5856 (3)	0.4680 (3)	0.1795 (2)	0.0360 (10)
N14	0.7079 (3)	0.5816 (3)	0.2175 (3)	0.0592 (13)
H14A	0.7406	0.6355	0.2039	0.050*
H14B	0.7447	0.5346	0.2464	0.050*
N21	0.7605 (3)	0.3845 (3)	0.3162 (2)	0.0342 (10)
N22	0.7372 (3)	0.4610 (3)	0.4359 (3)	0.0560 (13)
H22A	0.6780	0.4516	0.4208	0.050*
H22B	0.7610	0.4978	0.4839	0.050*
N23	0.7148 (2)	0.2931 (3)	0.1671 (2)	0.0333 (10)
N24	0.6186 (3)	0.2242 (3)	0.0405 (2)	0.0513 (13)
H24A	0.5788	0.2330	0.0664	0.050*
H24B	0.6009	0.1984	−0.0080	0.050*
N31	0.6342 (4)	0.0406 (4)	0.4158 (3)	0.0608 (14)
N41	0.8469 (4)	0.0572 (5)	0.8500 (4)	0.0764 (17)
O31	0.5826 (2)	0.3387 (3)	0.34990 (19)	0.0382 (8)
O32	0.6516 (2)	0.2056 (2)	0.3248 (2)	0.0390 (9)
O33	0.5692 (3)	0.0173 (3)	0.3555 (3)	0.0813 (14)
O34	0.7105 (4)	0.0015 (3)	0.4328 (3)	0.0918 (15)
O41	0.8915 (4)	0.0340 (4)	0.8015 (4)	0.125 (2)
O42	0.8355 (4)	0.0051 (4)	0.9037 (4)	0.121 (2)
O43	0.6322 (3)	0.0242 (3)	0.8000 (2)	0.0693 (12)
O44	0.6394 (2)	0.0765 (3)	0.9281 (2)	0.0442 (9)
S11	0.34324 (9)	0.22051 (12)	0.09485 (10)	0.0619 (5)

S12	0.54644 (11)	0.63624 (11)	0.10792 (10)	0.0639 (5)
S21	0.90877 (10)	0.45038 (12)	0.42205 (9)	0.0605 (5)
S22	0.80094 (10)	0.22774 (12)	0.06398 (9)	0.0600 (5)
C11	0.4490 (3)	0.3681 (4)	0.1231 (3)	0.0394 (13)
C12	0.3624 (3)	0.3435 (4)	0.0819 (3)	0.0579 (16)
H12	0.3182	0.3870	0.0503	0.070*
C13	0.4568 (3)	0.2098 (4)	0.1580 (3)	0.0377 (13)
C14	0.4950 (3)	0.4635 (4)	0.1267 (3)	0.0400 (13)
C15	0.4637 (4)	0.5468 (4)	0.0854 (3)	0.0578 (16)
H15	0.4045	0.5551	0.0490	0.069*
C16	0.6210 (4)	0.5546 (4)	0.1741 (3)	0.0440 (14)
C21	0.8340 (3)	0.3625 (4)	0.2837 (3)	0.0382 (13)
C22	0.9169 (3)	0.3941 (4)	0.3312 (3)	0.0503 (15)
H22	0.9714	0.3864	0.3169	0.060*
C23	0.7909 (3)	0.4301 (4)	0.3898 (3)	0.0389 (13)
C24	0.8087 (3)	0.3113 (4)	0.2028 (3)	0.0412 (14)
C25	0.8650 (4)	0.2812 (4)	0.1574 (3)	0.0518 (15)
H25	0.9288	0.2884	0.1740	0.062*
C26	0.7012 (3)	0.2497 (4)	0.0923 (3)	0.0400 (13)
C31	0.6186 (4)	0.1145 (5)	0.4751 (3)	0.0502 (15)
C32	0.6054 (3)	0.2126 (4)	0.4535 (3)	0.0430 (14)
C33	0.5913 (4)	0.2761 (5)	0.5137 (3)	0.0571 (16)
H33	0.5823	0.3428	0.5015	0.068*
C34	0.5903 (4)	0.2412 (6)	0.5924 (4)	0.077 (2)
H34	0.5817	0.2849	0.6328	0.093*
C35	0.6019 (5)	0.1430 (7)	0.6115 (5)	0.088 (3)
H35	0.5999	0.1202	0.6642	0.105*
C36	0.6164 (4)	0.0787 (5)	0.5530 (4)	0.0694 (19)
H36	0.6246	0.0120	0.5653	0.083*
C37	0.6130 (3)	0.2545 (4)	0.3705 (3)	0.0381 (13)
C41	0.7178 (3)	0.1665 (4)	0.8473 (3)	0.0381 (12)
C42	0.8047 (4)	0.1558 (4)	0.8383 (3)	0.0485 (14)
C43	0.8544 (4)	0.2328 (5)	0.8205 (4)	0.073 (2)
H43	0.9123	0.2219	0.8133	0.087*
C44	0.8183 (6)	0.3257 (5)	0.8131 (4)	0.081 (2)
H44	0.8523	0.3788	0.8027	0.097*
C45	0.7319 (5)	0.3402 (5)	0.8213 (4)	0.0709 (19)
H45	0.7062	0.4029	0.8150	0.085*
C46	0.6824 (4)	0.2605 (4)	0.8390 (3)	0.0541 (15)
H46	0.6242	0.2711	0.8454	0.065*
C47	0.6591 (3)	0.0811 (4)	0.8611 (3)	0.0382 (13)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni	0.0287 (3)	0.0303 (4)	0.0332 (4)	−0.0025 (3)	0.0066 (3)	−0.0019 (3)
N11	0.030 (2)	0.033 (3)	0.034 (2)	−0.002 (2)	0.0065 (18)	−0.004 (2)
N12	0.050 (3)	0.040 (3)	0.073 (3)	−0.010 (2)	0.010 (2)	0.002 (3)

N13	0.034 (2)	0.032 (3)	0.040 (2)	−0.003 (2)	0.0092 (19)	0.003 (2)
N14	0.048 (3)	0.039 (3)	0.085 (4)	−0.011 (2)	0.010 (3)	0.009 (3)
N21	0.032 (2)	0.036 (3)	0.032 (2)	−0.005 (2)	0.0042 (18)	−0.005 (2)
N22	0.057 (3)	0.061 (3)	0.046 (3)	−0.010 (3)	0.010 (2)	−0.021 (3)
N23	0.028 (2)	0.036 (3)	0.034 (2)	−0.0033 (19)	0.0062 (18)	0.001 (2)
N24	0.045 (3)	0.075 (4)	0.033 (2)	−0.007 (3)	0.010 (2)	−0.019 (2)
N31	0.074 (4)	0.041 (3)	0.056 (3)	−0.008 (3)	0.001 (3)	0.010 (3)
N41	0.051 (4)	0.086 (5)	0.098 (5)	−0.003 (3)	0.031 (3)	−0.015 (4)
O31	0.0360 (19)	0.036 (2)	0.044 (2)	0.0023 (18)	0.0133 (16)	−0.0016 (19)
O32	0.036 (2)	0.037 (2)	0.044 (2)	0.0014 (17)	0.0126 (16)	−0.0016 (18)
O33	0.097 (3)	0.057 (3)	0.068 (3)	−0.015 (3)	−0.010 (3)	0.000 (3)
O34	0.090 (4)	0.068 (3)	0.106 (4)	0.012 (3)	0.010 (3)	0.002 (3)
O41	0.117 (4)	0.109 (4)	0.188 (6)	−0.018 (4)	0.104 (4)	−0.047 (4)
O42	0.142 (5)	0.109 (5)	0.133 (5)	0.071 (4)	0.071 (4)	0.063 (4)
O43	0.100 (3)	0.066 (3)	0.054 (2)	−0.041 (3)	0.041 (2)	−0.021 (2)
O44	0.049 (2)	0.051 (2)	0.036 (2)	−0.0054 (19)	0.0173 (17)	0.0064 (19)
S11	0.0358 (8)	0.0717 (12)	0.0687 (10)	−0.0177 (8)	0.0004 (7)	−0.0052 (9)
S12	0.0767 (12)	0.0371 (9)	0.0722 (11)	0.0040 (8)	0.0130 (9)	0.0124 (9)
S21	0.0438 (9)	0.0706 (12)	0.0553 (9)	−0.0171 (8)	−0.0041 (7)	−0.0125 (9)
S22	0.0544 (10)	0.0708 (12)	0.0624 (10)	−0.0030 (9)	0.0287 (8)	−0.0206 (9)
C11	0.034 (3)	0.044 (4)	0.040 (3)	−0.001 (3)	0.009 (2)	−0.001 (3)
C12	0.035 (3)	0.064 (4)	0.065 (4)	−0.006 (3)	−0.001 (3)	0.001 (4)
C13	0.031 (3)	0.044 (4)	0.035 (3)	−0.006 (3)	0.005 (2)	−0.006 (3)
C14	0.039 (3)	0.042 (3)	0.037 (3)	0.005 (3)	0.008 (2)	0.005 (3)
C15	0.052 (4)	0.052 (4)	0.061 (4)	0.011 (3)	0.004 (3)	0.014 (3)
C16	0.053 (4)	0.033 (3)	0.050 (3)	−0.001 (3)	0.022 (3)	0.001 (3)
C21	0.029 (3)	0.044 (3)	0.039 (3)	−0.007 (2)	0.005 (2)	0.003 (3)
C22	0.032 (3)	0.061 (4)	0.058 (4)	−0.005 (3)	0.012 (3)	−0.005 (3)
C23	0.040 (3)	0.039 (3)	0.035 (3)	−0.006 (3)	0.007 (2)	0.003 (3)
C24	0.032 (3)	0.045 (4)	0.049 (3)	−0.002 (3)	0.015 (3)	−0.003 (3)
C25	0.044 (3)	0.052 (4)	0.059 (4)	−0.001 (3)	0.016 (3)	−0.004 (3)
C26	0.042 (3)	0.045 (4)	0.033 (3)	0.000 (3)	0.011 (2)	0.001 (3)
C31	0.049 (4)	0.061 (4)	0.037 (3)	−0.011 (3)	0.007 (3)	0.003 (3)
C32	0.042 (3)	0.049 (4)	0.038 (3)	−0.009 (3)	0.012 (2)	0.001 (3)
C33	0.064 (4)	0.068 (5)	0.044 (4)	−0.002 (3)	0.022 (3)	−0.004 (3)
C34	0.078 (5)	0.115 (7)	0.048 (4)	−0.019 (5)	0.034 (4)	−0.011 (5)
C35	0.084 (5)	0.123 (8)	0.054 (5)	−0.029 (5)	0.018 (4)	0.022 (5)
C36	0.071 (4)	0.074 (5)	0.058 (4)	−0.017 (4)	0.010 (4)	0.021 (4)
C37	0.030 (3)	0.040 (4)	0.042 (3)	−0.003 (3)	0.006 (2)	−0.002 (3)
C41	0.043 (3)	0.041 (3)	0.031 (3)	−0.009 (3)	0.010 (2)	−0.003 (3)
C42	0.041 (3)	0.050 (4)	0.057 (4)	−0.012 (3)	0.018 (3)	−0.007 (3)
C43	0.063 (4)	0.082 (5)	0.083 (5)	−0.037 (4)	0.037 (4)	−0.016 (5)
C44	0.116 (7)	0.057 (5)	0.087 (5)	−0.037 (5)	0.058 (5)	−0.003 (4)
C45	0.103 (6)	0.041 (4)	0.069 (4)	−0.005 (4)	0.025 (4)	0.005 (4)
C46	0.054 (4)	0.042 (4)	0.060 (4)	−0.001 (3)	0.008 (3)	0.003 (3)
C47	0.035 (3)	0.037 (3)	0.040 (3)	−0.007 (3)	0.008 (3)	−0.003 (3)

Geometric parameters (Å, °)

Ni—N11	2.073 (4)	S12—C15	1.707 (6)
Ni—N13	2.078 (4)	S12—C16	1.726 (5)
Ni—N21	2.073 (4)	S21—C22	1.716 (5)
Ni—N23	2.060 (4)	S21—C23	1.731 (5)
Ni—O31	2.143 (3)	S22—C25	1.723 (5)
Ni—O32	2.217 (3)	S22—C26	1.732 (5)
Ni—C37	2.500 (5)	C11—C12	1.332 (6)
N11—C13	1.314 (6)	C11—C14	1.466 (7)
N11—C11	1.388 (6)	C12—H12	0.9300
N12—C13	1.320 (6)	C14—C15	1.335 (6)
N12—H12A	0.7678	C15—H15	0.9300
N12—H12B	0.8257	C21—C22	1.342 (6)
N13—C16	1.307 (6)	C21—C24	1.453 (7)
N13—C14	1.396 (5)	C22—H22	0.9300
N14—C16	1.353 (6)	C24—C25	1.351 (6)
N14—H14A	0.9484	C25—H25	0.9300
N14—H14B	0.8884	C31—C32	1.379 (7)
N21—C23	1.320 (6)	C31—C36	1.381 (7)
N21—C21	1.399 (6)	C32—C33	1.378 (7)
N22—C23	1.332 (6)	C32—C37	1.516 (7)
N22—H22A	0.8674	C33—C34	1.384 (7)
N22—H22B	0.9161	C33—H33	0.9300
N23—C26	1.327 (5)	C34—C35	1.371 (9)
N23—C24	1.395 (5)	C34—H34	0.9300
N24—C26	1.339 (6)	C35—C36	1.365 (9)
N24—H24A	0.8425	C35—H35	0.9300
N24—H24B	0.8409	C36—H36	0.9300
N31—O33	1.220 (5)	C41—C42	1.375 (7)
N31—O34	1.229 (6)	C41—C46	1.377 (7)
N31—C31	1.468 (7)	C41—C47	1.518 (7)
N41—O42	1.185 (6)	C42—C43	1.370 (7)
N41—O41	1.228 (6)	C43—C44	1.367 (9)
N41—C42	1.472 (8)	C43—H43	0.9300
O31—C37	1.243 (5)	C44—C45	1.369 (8)
O32—C37	1.267 (5)	C44—H44	0.9300
O43—C47	1.240 (5)	C45—C46	1.396 (7)
O44—C47	1.225 (5)	C45—H45	0.9300
S11—C12	1.720 (6)	C46—H46	0.9300
S11—C13	1.738 (5)		
N23—Ni—N21	80.04 (15)	C14—C15—S12	111.3 (4)
N23—Ni—N11	101.07 (14)	C14—C15—H15	124.3
N21—Ni—N11	178.41 (16)	S12—C15—H15	124.3
N23—Ni—N13	98.01 (15)	N13—C16—N14	124.3 (5)
N21—Ni—N13	98.64 (15)	N13—C16—S12	114.6 (4)
N11—Ni—N13	80.09 (15)	N14—C16—S12	121.2 (4)
N23—Ni—O31	157.03 (14)	C22—C21—N21	115.0 (5)

N21—Ni—O31	89.64 (13)	C22—C21—C24	129.8 (5)
N11—Ni—O31	89.73 (13)	N21—C21—C24	115.2 (4)
N13—Ni—O31	103.83 (14)	C21—C22—S21	111.0 (4)
N23—Ni—O32	98.57 (14)	C21—C22—H22	124.5
N21—Ni—O32	87.37 (13)	S21—C22—H22	124.5
N11—Ni—O32	93.59 (14)	N21—C23—N22	124.3 (5)
N13—Ni—O32	163.11 (14)	N21—C23—S21	114.2 (4)
O31—Ni—O32	60.22 (12)	N22—C23—S21	121.4 (4)
N23—Ni—C37	128.30 (17)	C25—C24—N23	116.4 (5)
N21—Ni—C37	87.41 (15)	C25—C24—C21	127.7 (5)
N11—Ni—C37	92.77 (15)	N23—C24—C21	115.9 (4)
N13—Ni—C37	133.54 (17)	C24—C25—S22	109.8 (4)
O31—Ni—C37	29.82 (13)	C24—C25—H25	125.1
O32—Ni—C37	30.42 (13)	S22—C25—H25	125.1
C13—N11—C11	110.6 (4)	N23—C26—N24	124.8 (4)
C13—N11—Ni	134.5 (3)	N23—C26—S22	114.5 (4)
C11—N11—Ni	114.3 (3)	N24—C26—S22	120.7 (4)
C13—N12—H12A	119.7	C32—C31—C36	122.7 (6)
C13—N12—H12B	117.2	C32—C31—N31	121.9 (5)
H12A—N12—H12B	114.3	C36—C31—N31	115.4 (6)
C16—N13—C14	110.2 (4)	C33—C32—C31	117.4 (5)
C16—N13—Ni	135.8 (4)	C33—C32—C37	118.8 (5)
C14—N13—Ni	113.9 (3)	C31—C32—C37	123.6 (5)
C16—N14—H14A	125.4	C32—C33—C34	120.4 (6)
C16—N14—H14B	116.8	C32—C33—H33	119.8
H14A—N14—H14B	113.0	C34—C33—H33	119.8
C23—N21—C21	110.3 (4)	C35—C34—C33	120.9 (7)
C23—N21—Ni	135.4 (3)	C35—C34—H34	119.5
C21—N21—Ni	114.3 (3)	C33—C34—H34	119.5
C23—N22—H22A	122.8	C36—C35—C34	119.7 (7)
C23—N22—H22B	120.8	C36—C35—H35	120.1
H22A—N22—H22B	116.3	C34—C35—H35	120.1
C26—N23—C24	109.5 (4)	C35—C36—C31	118.9 (7)
C26—N23—Ni	136.0 (3)	C35—C36—H36	120.6
C24—N23—Ni	114.5 (3)	C31—C36—H36	120.6
C26—N24—H24A	108.4	O31—C37—O32	121.3 (5)
C26—N24—H24B	133.9	O31—C37—C32	118.2 (5)
H24A—N24—H24B	117.5	O32—C37—C32	120.5 (5)
O33—N31—O34	123.9 (6)	O31—C37—Ni	59.0 (3)
O33—N31—C31	118.1 (5)	O32—C37—Ni	62.3 (2)
O34—N31—C31	117.8 (5)	C32—C37—Ni	174.9 (4)
O42—N41—O41	124.0 (7)	C42—C41—C46	116.4 (5)
O42—N41—C42	119.3 (6)	C42—C41—C47	123.8 (5)
O41—N41—C42	116.7 (7)	C46—C41—C47	119.7 (5)
C37—O31—Ni	91.2 (3)	C43—C42—C41	123.1 (6)
C37—O32—Ni	87.2 (3)	C43—C42—N41	118.6 (6)
C12—S11—C13	89.0 (3)	C41—C42—N41	118.4 (5)
C15—S12—C16	89.1 (3)	C44—C43—C42	119.6 (6)
C22—S21—C23	89.4 (2)	C44—C43—H43	120.2

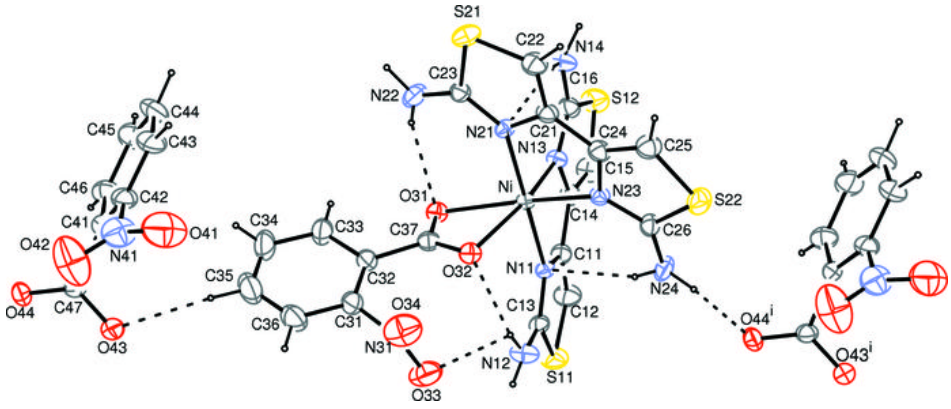
C25—S22—C26	89.8 (3)	C42—C43—H43	120.2
C12—C11—N11	115.5 (5)	C43—C44—C45	119.5 (6)
C12—C11—C14	129.0 (5)	C43—C44—H44	120.2
N11—C11—C14	115.5 (4)	C45—C44—H44	120.2
C11—C12—S11	110.9 (4)	C44—C45—C46	119.8 (6)
C11—C12—H12	124.5	C44—C45—H45	120.1
S11—C12—H12	124.5	C46—C45—H45	120.1
N11—C13—N12	124.8 (4)	C41—C46—C45	121.6 (6)
N11—C13—S11	113.9 (4)	C41—C46—H46	119.2
N12—C13—S11	121.3 (4)	C45—C46—H46	119.2
C15—C14—N13	114.8 (5)	O44—C47—O43	126.1 (5)
C15—C14—C11	129.5 (5)	O44—C47—C41	118.7 (5)
N13—C14—C11	115.7 (4)	O43—C47—C41	115.1 (5)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N12—H12A···O43^{i}	0.77	2.01	2.779 (6)	176
N12—H12B···O32	0.83	2.23	2.982 (6)	151
N12—H12B···O33	0.83	2.48	2.999 (6)	122
N14—H14A···O32^{ii}	0.95	2.06	2.953 (5)	156
N14—H14B···N21	0.89	2.32	3.114 (6)	149
N22—H22A···O31	0.87	2.20	2.886 (6)	136
N22—H22B···O44^{iii}	0.92	2.06	2.923 (6)	156
N24—H24A···N11	0.84	2.39	3.204 (5)	161
N24—H24B···O44^{iv}	0.84	2.13	2.810 (5)	137

Symmetry codes: (i) −*x*+1, −*y*, −*z*+1; (ii) −*x*+3/2, *y*+1/2, −*z*+1/2; (iii) −*x*+3/2, *y*+1/2, −*z*+3/2; (iv) *x*, *y*, *z*−1.

Fig. 1


S21
C22
N14
C23
C16
N22
S12
N21
C21
C24
C25
N13
C15
Ni
N23
S22
O31
C14
C26
C37
C33
C34
O41
O42
N41
C11
C35
C32
O32
N11
N24
O44i
C13
C12
C36
C31
O34
C45
C44
C43
C46
C42
C41
O44
C47
O43
N31
N12
S11
O33
O43i