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trans-Dipyridinebis(sulfamerazinato)-nickel(II)–pyridine (1/4)

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Key indicators

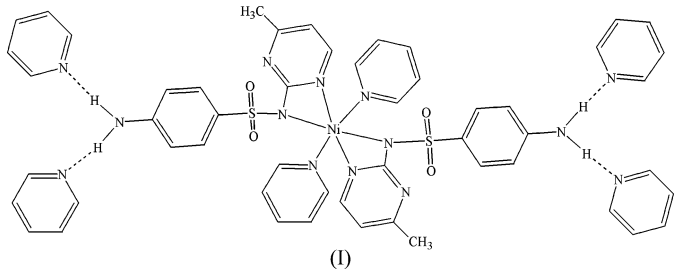
Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.004 Å
R factor = 0.053
wR factor = 0.143
Data-to-parameter ratio = 17.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $[Ni(C_{11}H_{11}N_4O_2S)_2(C_5H_5N)_2]\cdot 4C_5H_5N$, contains the centrosymmetric octahedral complex *trans*-$[Ni(smr)_2(py)_2]$ (where smr is the sulfamerazinate anion and py is pyridine) linked to four pyridine molecules *via* N—H···N hydrogen bonds. This is the first crystal structure of a metal complex of sulfamerazine.

Comment

The sulfamerazine molecule was introduced into medical therapy because, like many sulfonamide derivatives, it exhibits antibacterial activity. The presence of several potential donor sites, namely the amino, pyrimidine and sulfonamide N atoms and the sulfonyl O atoms, make this ligand a versatile complexing agent. Here, we report the structure of the title nickel complex, (I), of the sulfamerazinate anion (Fig. 1). This is the first crystal structure of a metal complex of sulfamerazine.



(I)

In complex (I), the Ni atom lies on a centre of inversion, and the complex contains two bidentate N-coordinated sulfamerazinate anions and two pyridine molecules occupying the *trans* sites. In addition, four pyridine molecules are linked *via* N—H···N hydrogen bonds to the terminal amino groups of the sulfamerazinate ligands (Table 1, Fig. 1).

The relative orientations of the sulfamerazinate ligands and the coordinated pyridine molecules are such that they are nearly perpendicular to each other. Such an orientation of the ligands around the Ni atom appears to be dictated more by steric considerations than any other factors.

The Ni—N bond distances involving the sulfonamide atom N11, the pyrimido atom N12 and the pyrimidine atom N1 are very similar, at 2.139 (2), 2.100 (2) and 2.080 (2) Å, respectively. The tetrahedral coordination at S is distorted, as also found in the neutral sulfamerazine molecule. The endocyclic angle at C11 in complex (I) is 125.2 (2)°, which is somewhat smaller than the corresponding values found in the various polymorphs of the free sulfamerazine molecule [127.5 (2) (Hossain, 2006), 127.1 (7) (Acharya *et al.*, 1982), and 127.1 (4)

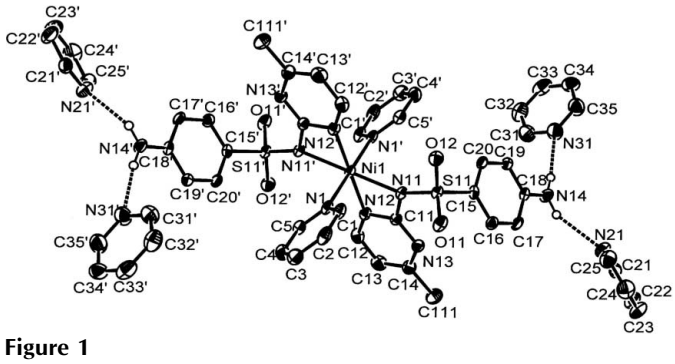


Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms bonded to C atoms have been omitted for clarity. Hydrogen bonds are shown as dashed lines. Atoms marked with a prime are at the symmetry position $(1-x, 1-y, 1-z)$.

and 128.2 (4)° (Caria & Mohamed, 1992)], due to the coordination to the Ni centre.

The S—O bond distances of 1.4460 (15) and 1.4435 (17) Å in (I) are longer than the corresponding bonds in pure sulfamerazine, where the values obtained are 1.4398 (16) and 1.4293 (17) Å (Hossain, 2006), 1.430 (6) and 1.441 (6) Å (Acharya *et al.*, 1982), and 1.424 (4) and 1.435 (3), and 1.414 (4) and 1.431 (3) Å (Caria & Mohamed, 1992).

The H atoms of the amino groups form intermolecular hydrogen bonds with the N atoms of four pyridine molecules (Table 1, Fig. 1).

Experimental

Solid sulfamerazine (Hsmr) (0.529 g, 2 mmol) was dissolved in hot methanol (50 ml) and a methanolic solution (10 ml) of $NiCl_2{\cdot}6H_2O$ (0.238 g, 1 mmol) was added slowly with constant stirring on a hot plate at 333 K. A pink precipitate formed and stirring of the mixture was continued for 6 h. The precipitate was then filtered off and dried over silica gel. The precipitate was dissolved in a mixture of pyridine and water (10 ml, 1:10 *v*/*v*) and stirred for 30 min. The solution was then filtered and left for crystallization, and a week later pale-violet block-shaped crystals of (I) were obtained. These were removed by filtration and dried over silica gel.

Crystal data

$[Ni(C_{11}H_{11}N_4O_2S)_2(C_5H_5N)_2]\cdot 4C_5H_5N$	$\gamma = 84.144\ (1)^\circ$
$M_r = 1059.91$	$V = 1311.85\ (5)$ Å^3
Triclinic, $P\overline{1}$	$Z = 1$
$a = 9.9781\ (2)$ Å	$D_x = 1.342$ Mg m^{-3}
$b = 10.0610\ (2)$ Å	Mo $K\alpha$ radiation
$c = 13.2582\ (4)$ Å	$\mu = 0.51$ mm^{-1}
$\alpha = 89.744\ (1)^\circ$	$T = 150\ (2)$ K
$\beta = 82.238\ (1)^\circ$	Block, pale violet
	0.18 × 0.16 × 0.06 mm

Data collection

Nonius KappaCCD area-detector diffractometer	24079 measured reflections
ω scans	5955 independent reflections
Absorption correction: multi-scan (Blessing, 1995)	4409 reflections with $I > 2\sigma(I)$
$T_{min} = 0.914$, $T_{max} = 0.970$	$R_{int} = 0.159$
	$\theta_{max} = 27.5^\circ$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.053$	$w = 1/[\sigma^2(F_o^2) + (0.0633P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.143$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.01$	$\Delta\rho_{max} = 0.50$ e Å^{-3}
5955 reflections	$\Delta\rho_{min} = -1.13$ e Å^{-3}
332 parameters	

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

D—H···A	D—H	H···A	D···A	D—H···A
N14—H14B···N31	0.88	2.15	3.029 (3)	173
N14—H14A···N21	0.88	2.33	3.067 (3)	141

All H atoms were treated as riding atoms, with C—H = 0.95 Å and N—H = 0.88 Å, and with $U_{iso}(H) = 1.2U_{eq}(C,N)$, or $1.5U_{eq}(C)$ for the methyl groups. The mosaicity of the compound was high, so R_{int} is 0.159. The deepest hole is located 0.90 Å from atom Ni1.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); 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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supporting information

Acta Cryst. (2006). E**62**, m2721–m2722 [https://doi.org/10.1107/S1600536806038116]

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$\gamma = 84.144$ (1)°
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$Z = 1$
$F(000) = 554$
$D_x = 1.342$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5955 reflections
$\theta = 2.9$–$27.5°$
$\mu = 0.51$ mm^{-1}
$T = 150$ K
Block, pale violet
0.18 × 0.16 × 0.06 mm

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Graphite monochromator
ω scans
Absorption correction: multi-scan (Blessing, 1995)
$T_{min} = 0.914$, $T_{max} = 0.970$
24079 measured reflections
5955 independent reflections
4409 reflections with $I > 2\sigma(I)$
$R_{int} = 0.159$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.0°$
$h = -12 \rightarrow 12$
$k = -13 \rightarrow 13$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.143$
$S = 1.01$
5955 reflections
332 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0633P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.50$ e Å^{-3}
$\Delta\rho_{min} = -1.13$ e Å^{-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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ni1	0.5000	0.5000	0.5000	0.01886 (14)
S11	0.30067 (5)	0.23831 (5)	0.59767 (4)	0.01937 (16)
O11	0.16033 (14)	0.27796 (16)	0.63779 (13)	0.0278 (4)
O12	0.32609 (16)	0.18289 (16)	0.49588 (13)	0.0284 (4)
N11	0.39181 (17)	0.36225 (17)	0.59441 (15)	0.0192 (4)
N12	0.48660 (17)	0.52862 (18)	0.65801 (15)	0.0212 (4)
N13	0.34288 (18)	0.40324 (18)	0.77429 (15)	0.0229 (4)
N14	0.5484 (2)	−0.11971 (19)	0.89210 (16)	0.0283 (5)
H14A	0.5107	−0.1201	0.9560	0.034*
H14B	0.6271	−0.1666	0.8732	0.034*
C11	0.4035 (2)	0.4301 (2)	0.68068 (18)	0.0189 (5)
C12	0.5123 (2)	0.6010 (2)	0.7359 (2)	0.0267 (5)
H12	0.5694	0.6709	0.7229	0.032*
C13	0.4576 (3)	0.5769 (3)	0.8355 (2)	0.0329 (6)
H13	0.4779	0.6276	0.8907	0.039*
C14	0.3726 (2)	0.4762 (2)	0.85134 (19)	0.0279 (5)
C15	0.3652 (2)	0.1200 (2)	0.68170 (18)	0.0206 (5)
C16	0.3004 (2)	0.1118 (2)	0.78086 (19)	0.0234 (5)
H16	0.2157	0.1629	0.8012	0.028*
C17	0.3597 (2)	0.0289 (2)	0.85028 (19)	0.0248 (5)
H17	0.3146	0.0234	0.9178	0.030*
C18	0.4849 (2)	−0.0465 (2)	0.82228 (18)	0.0217 (5)
C19	0.5467 (2)	−0.0405 (2)	0.72041 (18)	0.0223 (5)
H19	0.6299	−0.0935	0.6988	0.027*
C20	0.4869 (2)	0.0422 (2)	0.65170 (18)	0.0221 (5)
H20	0.5296	0.0457	0.5834	0.026*
C111	0.3049 (3)	0.4424 (3)	0.9551 (2)	0.0413 (7)
H11A	0.2062	0.4623	0.9583	0.062*
H11B	0.3376	0.4956	1.0067	0.062*
H11C	0.3267	0.3471	0.9680	0.062*
N1	0.32122 (17)	0.62698 (18)	0.50398 (15)	0.0208 (4)
C1	0.2067 (2)	0.5820 (2)	0.47984 (19)	0.0260 (5)
H1	0.2090	0.4906	0.4614	0.031*
C2	0.0869 (2)	0.6628 (3)	0.4808 (2)	0.0320 (6)
H2	0.0080	0.6273	0.4640	0.038*
C3	0.0825 (2)	0.7957 (3)	0.5065 (2)	0.0364 (7)
H3	0.0008	0.8534	0.5073	0.044*
C4	0.1997 (2)	0.8441 (2)	0.5313 (2)	0.0327 (6)
H4	0.1996	0.9354	0.5493	0.039*
C5	0.3167 (2)	0.7563 (2)	0.52921 (19)	0.0248 (5)

H5	0.3967	0.7891	0.5464	0.030*
N21	0.3414 (2)	−0.2171 (2)	1.06138 (17)	0.0350 (5)
C21	0.3501 (2)	−0.2256 (2)	1.1609 (2)	0.0293 (6)
H21	0.4374	−0.2268	1.1820	0.035*
C22	0.2408 (3)	−0.2326 (3)	1.2341 (2)	0.0420 (7)
H22	0.2520	−0.2374	1.3041	0.050*
C23	0.1137 (3)	−0.2327 (3)	1.2042 (3)	0.0496 (8)
H23	0.0357	−0.2385	1.2531	0.059*
C24	0.1019 (3)	−0.2243 (3)	1.1022 (3)	0.0455 (7)
H24	0.0156	−0.2236	1.0794	0.055*
C25	0.2177 (3)	−0.2168 (3)	1.0338 (2)	0.0407 (7)
H25	0.2089	−0.2110	0.9634	0.049*
N31	0.8222 (2)	−0.2661 (2)	0.8118 (2)	0.0446 (6)
C31	0.8988 (3)	−0.1658 (3)	0.8132 (3)	0.0470 (8)
H31	0.8547	−0.0790	0.8299	0.056*
C32	1.0387 (3)	−0.1806 (3)	0.7917 (3)	0.0470 (8)
H32	1.0895	−0.1060	0.7942	0.056*
C33	1.1028 (3)	−0.3059 (3)	0.7665 (2)	0.0465 (8)
H33	1.1989	−0.3191	0.7504	0.056*
C34	1.0269 (3)	−0.4113 (3)	0.7651 (2)	0.0431 (7)
H34	1.0688	−0.4991	0.7490	0.052*
C35	0.8869 (3)	−0.3863 (3)	0.7877 (3)	0.0459 (7)
H35	0.8339	−0.4593	0.7858	0.055*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0162 (2)	0.0220 (2)	0.0185 (2)	−0.00321 (15)	−0.00240 (16)	0.00663 (16)
S11	0.0182 (3)	0.0227 (3)	0.0185 (3)	−0.0055 (2)	−0.0044 (2)	0.0051 (2)
O11	0.0174 (8)	0.0374 (10)	0.0296 (10)	−0.0051 (7)	−0.0052 (7)	0.0114 (8)
O12	0.0352 (9)	0.0302 (9)	0.0216 (9)	−0.0076 (7)	−0.0079 (7)	0.0003 (7)
N11	0.0180 (9)	0.0217 (9)	0.0186 (10)	−0.0056 (7)	−0.0027 (7)	0.0045 (7)
N12	0.0179 (9)	0.0235 (10)	0.0223 (11)	−0.0025 (7)	−0.0030 (8)	0.0045 (8)
N13	0.0255 (10)	0.0238 (10)	0.0187 (11)	−0.0006 (8)	−0.0021 (8)	0.0034 (8)
N14	0.0291 (11)	0.0323 (11)	0.0211 (11)	0.0028 (8)	0.0001 (9)	0.0103 (9)
C11	0.0158 (10)	0.0206 (11)	0.0199 (12)	0.0012 (8)	−0.0036 (9)	0.0046 (9)
C12	0.0285 (12)	0.0241 (12)	0.0302 (15)	−0.0061 (9)	−0.0111 (11)	0.0012 (10)
C13	0.0409 (15)	0.0335 (14)	0.0263 (15)	−0.0037 (11)	−0.0116 (12)	−0.0059 (11)
C14	0.0345 (13)	0.0292 (13)	0.0196 (13)	0.0022 (10)	−0.0064 (10)	0.0052 (10)
C15	0.0240 (11)	0.0177 (11)	0.0217 (13)	−0.0066 (8)	−0.0059 (9)	0.0049 (9)
C16	0.0188 (11)	0.0247 (12)	0.0262 (14)	−0.0042 (9)	0.0003 (10)	0.0035 (10)
C17	0.0252 (12)	0.0270 (12)	0.0210 (13)	−0.0059 (9)	0.0032 (10)	0.0074 (10)
C18	0.0243 (11)	0.0195 (11)	0.0219 (13)	−0.0062 (9)	−0.0022 (10)	0.0066 (9)
C19	0.0234 (11)	0.0203 (11)	0.0223 (13)	−0.0015 (9)	−0.0003 (9)	0.0031 (9)
C20	0.0270 (12)	0.0214 (11)	0.0179 (12)	−0.0072 (9)	0.0002 (9)	0.0035 (9)
C111	0.0581 (18)	0.0446 (16)	0.0199 (15)	−0.0034 (13)	−0.0016 (13)	0.0037 (12)
N1	0.0171 (9)	0.0264 (10)	0.0193 (10)	−0.0039 (7)	−0.0031 (8)	0.0102 (8)
C1	0.0237 (12)	0.0305 (13)	0.0252 (14)	−0.0070 (9)	−0.0060 (10)	0.0114 (10)

C2	0.0200 (12)	0.0444 (15)	0.0332 (15)	−0.0080 (10)	−0.0067 (10)	0.0186 (12)
C3	0.0261 (13)	0.0399 (15)	0.0393 (17)	0.0095 (11)	0.0000 (12)	0.0130 (12)
C4	0.0322 (13)	0.0274 (13)	0.0368 (16)	0.0007 (10)	−0.0015 (11)	0.0079 (11)
C5	0.0236 (12)	0.0275 (12)	0.0240 (13)	−0.0056 (9)	−0.0031 (10)	0.0059 (10)
N21	0.0359 (12)	0.0426 (13)	0.0261 (13)	−0.0107 (10)	0.0018 (10)	0.0032 (10)
C21	0.0317 (13)	0.0248 (12)	0.0315 (15)	−0.0045 (10)	−0.0036 (11)	0.0038 (11)
C22	0.0467 (17)	0.0500 (17)	0.0277 (16)	−0.0077 (13)	0.0025 (13)	0.0107 (13)
C23	0.0403 (17)	0.0557 (19)	0.049 (2)	−0.0130 (14)	0.0151 (15)	0.0062 (15)
C24	0.0313 (15)	0.0487 (18)	0.058 (2)	−0.0070 (12)	−0.0087 (14)	0.0030 (15)
C25	0.0471 (16)	0.0464 (17)	0.0304 (16)	−0.0096 (13)	−0.0091 (13)	0.0043 (13)
N31	0.0311 (12)	0.0375 (13)	0.0620 (18)	0.0026 (10)	0.0003 (12)	0.0074 (12)
C31	0.0454 (17)	0.0402 (16)	0.052 (2)	0.0053 (13)	−0.0037 (15)	0.0046 (14)
C32	0.0431 (17)	0.0534 (19)	0.048 (2)	−0.0146 (14)	−0.0109 (14)	0.0127 (15)
C33	0.0261 (14)	0.071 (2)	0.0389 (18)	0.0060 (14)	−0.0019 (12)	0.0175 (15)
C34	0.0381 (16)	0.0478 (17)	0.0383 (18)	0.0132 (13)	−0.0008 (13)	0.0035 (13)
C35	0.0433 (16)	0.0387 (16)	0.055 (2)	0.0002 (12)	−0.0061 (14)	0.0058 (14)

Geometric parameters (Å, º)

Ni1—N1	2.0802 (18)	C111—H11C	0.9800
Ni1—N1^{i}	2.0802 (18)	N1—C5	1.339 (3)
Ni1—N12^{i}	2.100 (2)	N1—C1	1.348 (3)
Ni1—N12	2.100 (2)	C1—C2	1.374 (3)
Ni1—N11^{i}	2.1396 (18)	C1—H1	0.9500
Ni1—N11	2.1396 (18)	C2—C3	1.376 (4)
S11—O12	1.4429 (18)	C2—H2	0.9500
S11—O11	1.4456 (16)	C3—C4	1.390 (4)
S11—N11	1.6137 (18)	C3—H3	0.9500
S11—C15	1.760 (2)	C4—C5	1.388 (3)
N11—C11	1.359 (3)	C4—H4	0.9500
N12—C12	1.334 (3)	C5—H5	0.9500
N12—C11	1.364 (3)	N21—C25	1.334 (4)
N13—C14	1.343 (3)	N21—C21	1.336 (3)
N13—C11	1.344 (3)	C21—C22	1.366 (4)
N14—C18	1.363 (3)	C21—H21	0.9500
N14—H14A	0.8800	C22—C23	1.379 (4)
N14—H14B	0.8800	C22—H22	0.9500
C12—C13	1.389 (4)	C23—C24	1.374 (5)
C12—H12	0.9500	C23—H23	0.9500
C13—C14	1.383 (4)	C24—C25	1.377 (4)
C13—H13	0.9500	C24—H24	0.9500
C14—C111	1.502 (4)	C25—H25	0.9500
C15—C20	1.387 (3)	N31—C31	1.328 (4)
C15—C16	1.390 (3)	N31—C35	1.330 (3)
C16—C17	1.390 (3)	C31—C32	1.380 (4)
C16—H16	0.9500	C31—H31	0.9500
C17—C18	1.399 (3)	C32—C33	1.376 (4)
C17—H17	0.9500	C32—H32	0.9500

C18—C19	1.411 (3)	C33—C34	1.366 (4)
C19—C20	1.384 (3)	C33—H33	0.9500
C19—H19	0.9500	C34—C35	1.386 (4)
C20—H20	0.9500	C34—H34	0.9500
C111—H11A	0.9800	C35—H35	0.9500
C111—H11B	0.9800		

N1—Ni1—N1^{i}	180.000 (1)	C19—C20—H20	119.7
N1—Ni1—N12^{i}	92.01 (7)	C15—C20—H20	119.7
N1^{i}—Ni1—N12^{i}	87.99 (7)	C14—C111—H11A	109.5
N1—Ni1—N12	87.99 (7)	C14—C111—H11B	109.5
N1^{i}—Ni1—N12	92.01 (7)	H11A—C111—H11B	109.5
N12^{i}—Ni1—N12	180.000 (16)	C14—C111—H11C	109.5
N1—Ni1—N11^{i}	90.39 (7)	H11A—C111—H11C	109.5
N1^{i}—Ni1—N11^{i}	89.61 (7)	H11B—C111—H11C	109.5
N12^{i}—Ni1—N11^{i}	63.36 (7)	C5—N1—C1	117.95 (19)
N12—Ni1—N11^{i}	116.64 (7)	C5—N1—Ni1	121.08 (15)
N1—Ni1—N11	89.61 (7)	C1—N1—Ni1	120.96 (15)
N1^{i}—Ni1—N11	90.39 (7)	N1—C1—C2	122.8 (2)
N12^{i}—Ni1—N11	116.64 (7)	N1—C1—H1	118.6
N12—Ni1—N11	63.36 (7)	C2—C1—H1	118.6
N11^{i}—Ni1—N11	180.00 (7)	C1—C2—C3	119.2 (2)
O12—S11—O11	116.66 (10)	C1—C2—H2	120.4
O12—S11—N11	104.95 (10)	C3—C2—H2	120.4
O11—S11—N11	111.73 (10)	C2—C3—C4	118.8 (2)
O12—S11—C15	108.81 (10)	C2—C3—H3	120.6
O11—S11—C15	107.21 (10)	C4—C3—H3	120.6
N11—S11—C15	107.11 (10)	C5—C4—C3	118.7 (2)
C11—N11—S11	121.07 (16)	C5—C4—H4	120.7
C11—N11—Ni1	92.33 (13)	C3—C4—H4	120.7
S11—N11—Ni1	146.00 (12)	N1—C5—C4	122.6 (2)
C12—N12—C11	116.8 (2)	N1—C5—H5	118.7
C12—N12—Ni1	148.88 (16)	C4—C5—H5	118.7
C11—N12—Ni1	93.91 (14)	C25—N21—C21	116.8 (2)
C14—N13—C11	116.5 (2)	N21—C21—C22	123.9 (3)
C18—N14—H14A	120.0	N21—C21—H21	118.0
C18—N14—H14B	120.0	C22—C21—H21	118.0
H14A—N14—H14B	120.0	C21—C22—C23	118.5 (3)
N13—C11—N11	125.0 (2)	C21—C22—H22	120.7
N13—C11—N12	125.2 (2)	C23—C22—H22	120.7
N11—C11—N12	109.76 (19)	C24—C23—C22	118.8 (3)
N12—C12—C13	121.6 (2)	C24—C23—H23	120.6
N12—C12—H12	119.2	C22—C23—H23	120.6
C13—C12—H12	119.2	C23—C24—C25	118.7 (3)
C14—C13—C12	117.6 (2)	C23—C24—H24	120.7
C14—C13—H13	121.2	C25—C24—H24	120.7
C12—C13—H13	121.2	N21—C25—C24	123.4 (3)
N13—C14—C13	122.1 (2)	N21—C25—H25	118.3

N13—C14—C111	115.2 (2)	C24—C25—H25	118.3
C13—C14—C111	122.7 (2)	C31—N31—C35	116.7 (2)
C20—C15—C16	119.7 (2)	N31—C31—C32	123.7 (3)
C20—C15—S11	119.92 (17)	N31—C31—H31	118.1
C16—C15—S11	120.13 (16)	C32—C31—H31	118.1
C17—C16—C15	120.0 (2)	C33—C32—C31	118.3 (3)
C17—C16—H16	120.0	C33—C32—H32	120.9
C15—C16—H16	120.0	C31—C32—H32	120.9
C16—C17—C18	121.0 (2)	C34—C33—C32	119.4 (3)
C16—C17—H17	119.5	C34—C33—H33	120.3
C18—C17—H17	119.5	C32—C33—H33	120.3
N14—C18—C17	121.1 (2)	C33—C34—C35	118.0 (3)
N14—C18—C19	120.7 (2)	C33—C34—H34	121.0
C17—C18—C19	118.2 (2)	C35—C34—H34	121.0
C20—C19—C18	120.4 (2)	N31—C35—C34	123.9 (3)
C20—C19—H19	119.8	N31—C35—H35	118.0
C18—C19—H19	119.8	C34—C35—H35	118.0
C19—C20—C15	120.6 (2)		

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N14—H14*B*···N31	0.88	2.15	3.029 (3)	173
N14—H14*A*···N21	0.88	2.33	3.067 (3)	141