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Bis(tetra-*n*-butylammonium) bis(5,6-dicyanopyrazine-2,3-dithiolato-κ^2S,S')nickelate(II)

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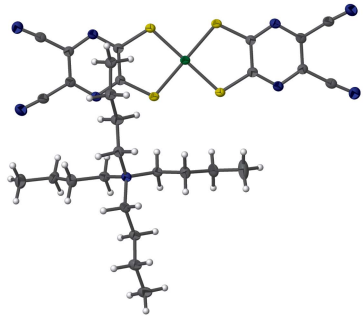
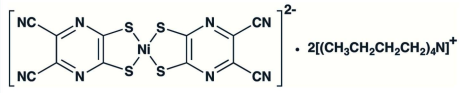
Structural data: full structural data are available from iucrdata.iucr.org

In the title salt, $(C_{16}H_{36}N)_2[Ni(C_6N_4S_2)_2]$, the centrosymmetric complex dianion is planar, with an r.m.s. deviation of 0.031 (1) Å. The Ni^{II} atom, lying on an inversion centre, has an almost undistorted square-planar coordination geometry, with Ni—S bond lengths of 2.1606 (5) and 2.1759 (5) Å.

3D view



Chemical scheme



Structure description

Metal dithiolene complexes have been widely investigated as conducting, magnetic or nonlinear optical materials (Cassoux *et al.*, 1991; Robertson & Cronin, 2002). Dithiolene ligands including the 2,3-dicyano-5,6-dimercaptopyrazine (dcdmp) moiety have extended π-conjugated systems and are expected to coordinate to transition metals, constructing organometallic coordination polymers (Nomura *et al.*, 2009; Rabaça & Almeida, 2010). In addition, intermolecular S···N and S···S contacts involving peripheral S and N atoms of these ligands may lead to the formation of unique molecular networks (Yamashita & Tomura, 1998). Three tetrabutylammonium salts of such $[M(dcdmp)_2]^{2-}$ complexes have been reported, where M = Au (Belo *et al.*, 2004), Pd (Tomura & Yamashita, 2012) and Cu (Belo *et al.*, 2005). Only one example (Belo *et al.*, 2006) of the $[Ni(dcdmp)_2]^{2-}$ complex anion with two dithiopheno-tetrathiafulvalenium as counter cations, was found in the Cambridge Structural Database (CSD, Version 5.38; Groom *et al.*, 2016). The molecular and crystal structures of the title Ni complex with tetra-*n*-butylammonium counter-cations is reported here.

The title salt, $[NBu_4]_2[Ni(dcdmp)_2]$, crystallizes in the space group $P\overline{1}$ and is isostructural with $[NBu_4]_2[Pd(dcdmp)_2]$ and $[NBu_4]_2[Cu(dcdmp)_2]$. The molecular structure of the complex dianion is shown in Fig. 1. The dianion is a flat molecule with an r.m.s. deviation of 0.031 (1) Å from the least-squares plane. The $Ni1^{II}$ atom lies on an inversion center and has a square-planar coordination sphere. The Ni1—S1 and Ni1—S2 distances and the S1—Ni1—S2 angle are 2.1606 (5), 2.1759 (5) Å and 91.72 (2)°,

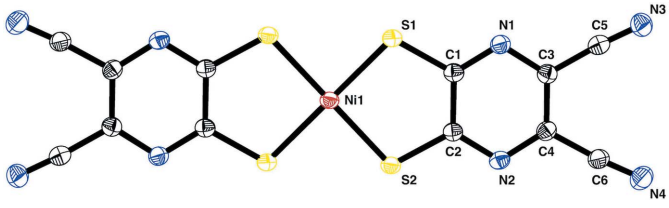


Figure 1
The molecular structure of the complex dianion in the title salt, with the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Unlabelled atoms are related to the labeled atoms by $(-x+1, -y, -z)$.

respectively. These values are comparable to those found in the salt bis(tetra-*n*-butylammonium) bis(4,5-dicyanobenzene-1,2-dithiolato-S,*S*′)nickelate(II) (Simão *et al.*, 2001). Fig. 2 shows the packing diagram of the title complex in a view along the *a* axis. The dianionic molecules form a layered structure parallel to (011) with an interlayer distance of *ca* 6.1 Å. The ordered tetra-*n*-butylammonium cations are inserted between these layers. Apart from Coulombic interactions, they are bound to the anions through weak C—H···N and C—H···S interactions (Table 1).

Synthesis and crystallization

The title complex was synthesized according to a literature protocol (Tomura *et al.*, 1994). Red crystals suitable for X-ray analysis were grown from an acetone solution.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Five reflections were omitted due to a poor agreement between observed and calculated intensities.

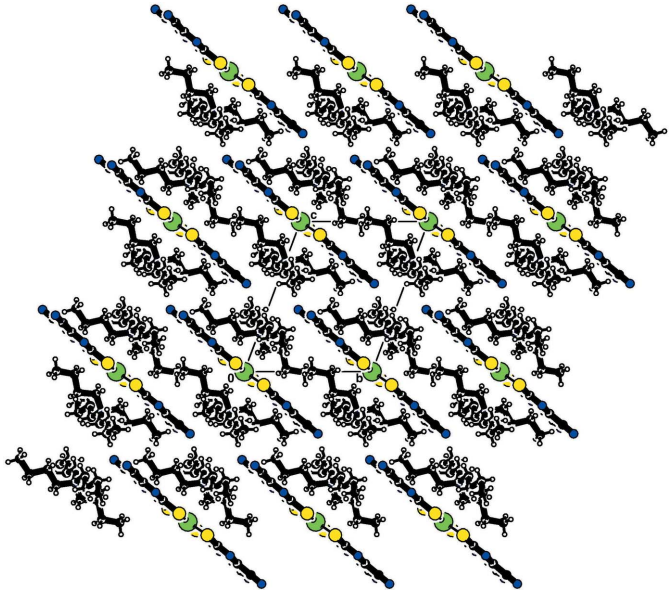


Figure 2
The crystal packing of the title complex, in a view along the *a* axis.

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

D—H···A	D—H	H···A	D···A	D—H···A
C15—H15A···N4^{i}	0.99	2.59	3.559 (3)	166
C13—H13A···S1^{ii}	0.99	2.82	3.748 (2)	157

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Ni(C_6N_4S_2)_2]\cdot 2C_{16}H_{36}N$
M_r	928.05
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	123
a, b, c (Å)	9.8217 (15), 10.5369 (15), 12.974 (2)
α, β, γ (°)	69.438 (4), 88.102 (7), 79.086 (7)
V (Å^3)	1233.6 (3)
Z	1
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.60
Crystal size (mm)	0.20 × 0.20 × 0.07
Data collection	
Diffractometer	Rigaku/MSC Mercury CCD
Absorption correction	–
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11061, 6629, 4998
R_{int}	0.034
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.725
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.046, 0.103, 0.99
No. of reflections	6629
No. of parameters	272
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.95, −0.53

Computer programs: *CrystalClear* (Rigaku/MSC, 2006), *SIR2014* (Burla *et al.*, 2015), *SHELXL2016* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x171059 [https://doi.org/10.1107/S2414314617010598]

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Crystal data

$[Ni(C_6N_4S_2)_2]\cdot 2C_{16}H_{36}N$
M_r = 928.05
Triclinic, $P\overline{1}$
a = 9.8217 (15) Å
b = 10.5369 (15) Å
c = 12.974 (2) Å
α = 69.438 (4)°
β = 88.102 (7)°
γ = 79.086 (7)°
V = 1233.6 (3) Å^3
Z = 1
$F(000)$ = 498
D_x = 1.249 Mg m^{-3}
Melting point: 516 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3425 reflections
θ = 1.7–30.7°
μ = 0.60 mm^{-1}
T = 123 K
Block, red
0.20 × 0.20 × 0.07 mm

Data collection

Rigaku/MSC Mercury CCD diffractometer
Radiation source: Rotating Anode
Graphite Monochromator monochromator
Detector resolution: 14.7059 pixels mm^{-1}
φ & ω scans
11061 measured reflections
6629 independent reflections
4998 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 31.0°, θ_{min} = 2.1°
h = −11→13
k = −14→10
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.103
S = 0.99
6629 reflections
272 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
$w = 1/[\sigma^2(F_o^2) + (0.0426P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.95 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-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.

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.500000	0.000000	0.000000	0.02062 (10)
S1	0.43264 (4)	−0.19178 (5)	0.08875 (4)	0.02579 (12)
S2	0.71462 (4)	−0.09135 (5)	0.05557 (4)	0.02277 (12)
N1	0.56827 (13)	−0.42938 (16)	0.22516 (13)	0.0237 (3)
N2	0.82580 (13)	−0.33856 (16)	0.19614 (13)	0.0232 (3)
N3	0.68291 (15)	−0.75826 (18)	0.41323 (15)	0.0321 (4)
N4	1.02495 (16)	−0.64124 (18)	0.37563 (17)	0.0388 (5)
N5	1.03854 (13)	−0.00072 (15)	0.26233 (12)	0.0195 (3)
C1	0.57891 (16)	−0.30369 (19)	0.15852 (15)	0.0216 (4)
C2	0.71003 (16)	−0.25614 (19)	0.14286 (15)	0.0206 (4)
C3	0.68651 (17)	−0.51067 (19)	0.27881 (16)	0.0232 (4)
C4	0.81279 (16)	−0.46538 (19)	0.26411 (16)	0.0233 (4)
C5	0.67992 (17)	−0.6480 (2)	0.35339 (16)	0.0255 (4)
C6	0.93412 (17)	−0.5598 (2)	0.32513 (17)	0.0267 (4)
C7	0.92689 (16)	−0.02356 (19)	0.34742 (15)	0.0224 (4)
H7A	0.971982	−0.080747	0.420318	0.027*
H7B	0.882538	0.066986	0.351566	0.027*
C8	0.81482 (17)	−0.0924 (2)	0.32549 (16)	0.0274 (4)
H8A	0.857409	−0.185325	0.325254	0.033*
H8B	0.770971	−0.037680	0.251702	0.033*
C9	0.70374 (17)	−0.1061 (2)	0.41151 (16)	0.0262 (4)
H9A	0.664389	−0.013924	0.414730	0.031*
H9B	0.746312	−0.165477	0.484817	0.031*
C10	0.58770 (17)	−0.1685 (2)	0.38420 (17)	0.0300 (5)
H10A	0.546505	−0.110648	0.311117	0.045*
H10B	0.516341	−0.173261	0.439346	0.045*
H10C	0.625754	−0.261643	0.384623	0.045*
C11	1.10593 (16)	−0.13536 (19)	0.24719 (15)	0.0220 (4)
H11A	1.034274	−0.168962	0.217291	0.026*
H11B	1.177309	−0.115180	0.191104	0.026*
C12	1.17300 (19)	−0.2504 (2)	0.34874 (16)	0.0291 (4)
H12A	1.104604	−0.269697	0.407353	0.035*
H12B	1.251077	−0.222371	0.376235	0.035*
C13	1.22608 (18)	−0.37964 (19)	0.32113 (17)	0.0283 (4)
H13A	1.293657	−0.358989	0.262000	0.034*
H13B	1.147464	−0.406106	0.292897	0.034*
C14	1.2952 (2)	−0.5005 (2)	0.42034 (19)	0.0389 (5)
H14A	1.374550	−0.475724	0.447544	0.058*
H14B	1.327294	−0.581133	0.398648	0.058*
H14C	1.228258	−0.522548	0.478674	0.058*

C15	1.14395 (15)	0.06092 (19)	0.30399 (15)	0.0216 (4)
H15A	1.093843	0.142392	0.319946	0.026*
H15B	1.186712	−0.007884	0.374330	0.026*
C16	1.25914 (16)	0.1048 (2)	0.22618 (15)	0.0239 (4)
H16A	1.218041	0.169146	0.153724	0.029*
H16B	1.316123	0.022741	0.215139	0.029*
C17	1.35122 (17)	0.1753 (2)	0.27221 (16)	0.0280 (4)
H17A	1.294010	0.257013	0.283628	0.034*
H17B	1.392453	0.110749	0.344569	0.034*
C18	1.46686 (18)	0.2203 (2)	0.19447 (17)	0.0332 (5)
H18A	1.527854	0.138786	0.187578	0.050*
H18B	1.520714	0.270043	0.223996	0.050*
H18C	1.426348	0.281070	0.121852	0.050*
C19	0.97771 (16)	0.09409 (18)	0.14931 (14)	0.0207 (4)
H19A	1.053150	0.099901	0.096272	0.025*
H19B	0.908733	0.050265	0.127099	0.025*
C20	0.90824 (17)	0.24005 (19)	0.13793 (16)	0.0259 (4)
H20A	0.972528	0.284576	0.164663	0.031*
H20B	0.824282	0.238287	0.182414	0.031*
C21	0.86853 (19)	0.3212 (2)	0.01593 (16)	0.0310 (5)
H21A	0.953720	0.323276	−0.027134	0.037*
H21B	0.808267	0.272688	−0.010449	0.037*
C22	0.7933 (2)	0.4686 (2)	−0.0051 (2)	0.0516 (7)
H22A	0.709623	0.467493	0.038254	0.077*
H22B	0.767219	0.514238	−0.083597	0.077*
H22C	0.854576	0.519104	0.016460	0.077*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.01826 (16)	0.02469 (19)	0.01825 (19)	−0.00601 (12)	0.00173 (12)	−0.00582 (15)
S1	0.0190 (2)	0.0269 (3)	0.0277 (3)	−0.00663 (17)	0.00041 (17)	−0.0037 (2)
S2	0.0193 (2)	0.0276 (3)	0.0200 (2)	−0.00756 (17)	0.00133 (17)	−0.0051 (2)
N1	0.0212 (7)	0.0251 (9)	0.0248 (9)	−0.0045 (6)	0.0014 (6)	−0.0087 (7)
N2	0.0194 (7)	0.0274 (9)	0.0236 (9)	−0.0042 (6)	0.0027 (6)	−0.0102 (7)
N3	0.0341 (8)	0.0265 (10)	0.0358 (11)	−0.0056 (7)	0.0003 (7)	−0.0111 (8)
N4	0.0294 (8)	0.0315 (10)	0.0534 (13)	−0.0031 (7)	−0.0063 (8)	−0.0132 (10)
N5	0.0183 (6)	0.0228 (8)	0.0174 (8)	−0.0036 (5)	0.0011 (5)	−0.0073 (7)
C1	0.0221 (8)	0.0257 (10)	0.0183 (9)	−0.0057 (7)	0.0030 (7)	−0.0091 (8)
C2	0.0210 (8)	0.0235 (9)	0.0186 (9)	−0.0043 (7)	0.0035 (6)	−0.0093 (8)
C3	0.0233 (8)	0.0239 (10)	0.0235 (10)	−0.0047 (7)	0.0028 (7)	−0.0097 (8)
C4	0.0217 (8)	0.0244 (10)	0.0249 (10)	−0.0028 (7)	0.0008 (7)	−0.0110 (8)
C5	0.0222 (8)	0.0294 (11)	0.0271 (11)	−0.0048 (7)	0.0015 (7)	−0.0128 (9)
C6	0.0226 (8)	0.0262 (10)	0.0329 (11)	−0.0053 (7)	0.0022 (8)	−0.0120 (9)
C7	0.0217 (8)	0.0255 (10)	0.0198 (10)	−0.0026 (7)	0.0040 (7)	−0.0089 (8)
C8	0.0244 (8)	0.0372 (12)	0.0237 (10)	−0.0090 (8)	0.0056 (7)	−0.0132 (9)
C9	0.0241 (8)	0.0273 (11)	0.0267 (11)	−0.0041 (7)	0.0056 (7)	−0.0096 (9)
C10	0.0262 (9)	0.0314 (11)	0.0284 (11)	−0.0070 (8)	0.0047 (8)	−0.0051 (9)

C11	0.0200 (8)	0.0246 (10)	0.0233 (10)	−0.0032 (7)	0.0030 (7)	−0.0118 (8)
C12	0.0318 (9)	0.0265 (11)	0.0270 (11)	0.0011 (8)	−0.0025 (8)	−0.0101 (9)
C13	0.0329 (9)	0.0207 (10)	0.0284 (11)	−0.0056 (7)	0.0082 (8)	−0.0054 (9)
C14	0.0421 (11)	0.0262 (11)	0.0424 (14)	0.0005 (9)	−0.0006 (10)	−0.0080 (11)
C15	0.0199 (8)	0.0251 (10)	0.0212 (10)	−0.0028 (7)	−0.0021 (7)	−0.0104 (8)
C16	0.0213 (8)	0.0301 (10)	0.0223 (10)	−0.0056 (7)	−0.0001 (7)	−0.0111 (9)
C17	0.0260 (9)	0.0361 (12)	0.0266 (11)	−0.0081 (8)	0.0002 (7)	−0.0156 (9)
C18	0.0287 (9)	0.0454 (13)	0.0313 (12)	−0.0152 (8)	0.0013 (8)	−0.0163 (11)
C19	0.0196 (7)	0.0261 (10)	0.0162 (9)	−0.0052 (7)	0.0008 (6)	−0.0068 (8)
C20	0.0267 (8)	0.0266 (10)	0.0226 (10)	−0.0017 (7)	−0.0008 (7)	−0.0080 (9)
C21	0.0336 (10)	0.0302 (11)	0.0243 (11)	−0.0013 (8)	−0.0063 (8)	−0.0053 (9)
C22	0.0662 (15)	0.0362 (14)	0.0351 (14)	0.0136 (11)	−0.0079 (12)	−0.0025 (12)

Geometric parameters (Å, º)

Ni1—S1	2.1606 (5)	C11—H11B	0.9900
Ni1—S1^{i}	2.1607 (5)	C12—C13	1.522 (3)
Ni1—S2	2.1759 (5)	C12—H12A	0.9900
Ni1—S2^{i}	2.1759 (5)	C12—H12B	0.9900
S1—C1	1.7229 (17)	C13—C14	1.523 (3)
S2—C2	1.7159 (19)	C13—H13A	0.9900
N1—C1	1.325 (2)	C13—H13B	0.9900
N1—C3	1.351 (2)	C14—H14A	0.9800
N2—C2	1.335 (2)	C14—H14B	0.9800
N2—C4	1.345 (2)	C14—H14C	0.9800
N3—C5	1.144 (2)	C15—C16	1.519 (2)
N4—C6	1.147 (2)	C15—H15A	0.9900
N5—C19	1.519 (2)	C15—H15B	0.9900
N5—C7	1.521 (2)	C16—C17	1.526 (2)
N5—C15	1.525 (2)	C16—H16A	0.9900
N5—C11	1.523 (2)	C16—H16B	0.9900
C1—C2	1.451 (2)	C17—C18	1.525 (2)
C3—C4	1.395 (2)	C17—H17A	0.9900
C3—C5	1.443 (3)	C17—H17B	0.9900
C4—C6	1.448 (2)	C18—H18A	0.9800
C7—C8	1.512 (2)	C18—H18B	0.9800
C7—H7A	0.9900	C18—H18C	0.9800
C7—H7B	0.9900	C19—C20	1.517 (2)
C8—C9	1.524 (2)	C19—H19A	0.9900
C8—H8A	0.9900	C19—H19B	0.9900
C8—H8B	0.9900	C20—C21	1.534 (3)
C9—C10	1.527 (3)	C20—H20A	0.9900
C9—H9A	0.9900	C20—H20B	0.9900
C9—H9B	0.9900	C21—C22	1.521 (3)
C10—H10A	0.9800	C21—H21A	0.9900
C10—H10B	0.9800	C21—H21B	0.9900
C10—H10C	0.9800	C22—H22A	0.9800
C11—C12	1.507 (3)	C22—H22B	0.9800

C11—H11A	0.9900	C22—H22C	0.9800
S1—Ni1—S1^{i}	180.0	C11—C12—H12B	109.8
S1—Ni1—S2	91.724 (19)	C13—C12—H12B	109.8
S1^{i}—Ni1—S2	88.275 (19)	H12A—C12—H12B	108.2
S1—Ni1—S2^{i}	88.275 (19)	C12—C13—C14	112.47 (17)
S1^{i}—Ni1—S2^{i}	91.725 (19)	C12—C13—H13A	109.1
S2—Ni1—S2^{i}	180.0	C14—C13—H13A	109.1
C1—S1—Ni1	105.40 (6)	C12—C13—H13B	109.1
C2—S2—Ni1	104.96 (6)	C14—C13—H13B	109.1
C1—N1—C3	116.12 (15)	H13A—C13—H13B	107.8
C2—N2—C4	116.28 (14)	C13—C14—H14A	109.5
C19—N5—C7	111.36 (12)	C13—C14—H14B	109.5
C19—N5—C15	111.42 (13)	H14A—C14—H14B	109.5
C7—N5—C15	106.35 (13)	C13—C14—H14C	109.5
C19—N5—C11	105.17 (13)	H14A—C14—H14C	109.5
C7—N5—C11	111.23 (13)	H14B—C14—H14C	109.5
C15—N5—C11	111.41 (12)	C16—C15—N5	115.56 (14)
N1—C1—C2	122.13 (15)	C16—C15—H15A	108.4
N1—C1—S1	119.28 (13)	N5—C15—H15A	108.4
C2—C1—S1	118.59 (14)	C16—C15—H15B	108.4
N2—C2—C1	120.75 (16)	N5—C15—H15B	108.4
N2—C2—S2	120.08 (13)	H15A—C15—H15B	107.5
C1—C2—S2	119.17 (13)	C15—C16—C17	110.93 (15)
N1—C3—C4	121.96 (17)	C15—C16—H16A	109.5
N1—C3—C5	118.20 (15)	C17—C16—H16A	109.5
C4—C3—C5	119.84 (16)	C15—C16—H16B	109.5
N2—C4—C3	122.75 (15)	C17—C16—H16B	109.5
N2—C4—C6	119.19 (15)	H16A—C16—H16B	108.0
C3—C4—C6	118.05 (17)	C18—C17—C16	111.35 (16)
N3—C5—C3	176.02 (18)	C18—C17—H17A	109.4
N4—C6—C4	175.5 (2)	C16—C17—H17A	109.4
C8—C7—N5	115.26 (15)	C18—C17—H17B	109.4
C8—C7—H7A	108.5	C16—C17—H17B	109.4
N5—C7—H7A	108.5	H17A—C17—H17B	108.0
C8—C7—H7B	108.5	C17—C18—H18A	109.5
N5—C7—H7B	108.5	C17—C18—H18B	109.5
H7A—C7—H7B	107.5	H18A—C18—H18B	109.5
C7—C8—C9	112.11 (16)	C17—C18—H18C	109.5
C7—C8—H8A	109.2	H18A—C18—H18C	109.5
C9—C8—H8A	109.2	H18B—C18—H18C	109.5
C7—C8—H8B	109.2	C20—C19—N5	117.09 (15)
C9—C8—H8B	109.2	C20—C19—H19A	108.0
H8A—C8—H8B	107.9	N5—C19—H19A	108.0
C8—C9—C10	111.19 (16)	C20—C19—H19B	108.0
C8—C9—H9A	109.4	N5—C19—H19B	108.0
C10—C9—H9A	109.4	H19A—C19—H19B	107.3
C8—C9—H9B	109.4	C19—C20—C21	108.27 (16)

C10—C9—H9B	109.4	C19—C20—H20A	110.0
H9A—C9—H9B	108.0	C21—C20—H20A	110.0
C9—C10—H10A	109.5	C19—C20—H20B	110.0
C9—C10—H10B	109.5	C21—C20—H20B	110.0
H10A—C10—H10B	109.5	H20A—C20—H20B	108.4
C9—C10—H10C	109.5	C22—C21—C20	112.99 (18)
H10A—C10—H10C	109.5	C22—C21—H21A	109.0
H10B—C10—H10C	109.5	C20—C21—H21A	109.0
C12—C11—N5	116.35 (15)	C22—C21—H21B	109.0
C12—C11—H11A	108.2	C20—C21—H21B	109.0
N5—C11—H11A	108.2	H21A—C21—H21B	107.8
C12—C11—H11B	108.2	C21—C22—H22A	109.5
N5—C11—H11B	108.2	C21—C22—H22B	109.5
H11A—C11—H11B	107.4	H22A—C22—H22B	109.5
C11—C12—C13	109.60 (16)	C21—C22—H22C	109.5
C11—C12—H12A	109.8	H22A—C22—H22C	109.5
C13—C12—H12A	109.8	H22B—C22—H22C	109.5

C3—N1—C1—C2	0.7 (3)	C19—N5—C7—C8	61.82 (19)
C3—N1—C1—S1	−178.76 (14)	C15—N5—C7—C8	−176.62 (15)
Ni1—S1—C1—N1	176.83 (13)	C11—N5—C7—C8	−55.14 (19)
Ni1—S1—C1—C2	−2.61 (16)	N5—C7—C8—C9	−177.56 (14)
C4—N2—C2—C1	−0.3 (3)	C7—C8—C9—C10	176.84 (16)
C4—N2—C2—S2	179.10 (13)	C19—N5—C11—C12	−178.87 (14)
N1—C1—C2—N2	−0.2 (3)	C7—N5—C11—C12	−58.20 (19)
S1—C1—C2—N2	179.21 (14)	C15—N5—C11—C12	60.28 (19)
N1—C1—C2—S2	−179.64 (14)	N5—C11—C12—C13	176.10 (14)
S1—C1—C2—S2	−0.2 (2)	C11—C12—C13—C14	−179.93 (15)
Ni1—S2—C2—N2	−176.53 (13)	C19—N5—C15—C16	−53.08 (18)
Ni1—S2—C2—C1	2.90 (15)	C7—N5—C15—C16	−174.61 (14)
C1—N1—C3—C4	−0.6 (3)	C11—N5—C15—C16	64.03 (19)
C1—N1—C3—C5	179.27 (16)	N5—C15—C16—C17	175.43 (14)
C2—N2—C4—C3	0.4 (3)	C15—C16—C17—C18	−179.76 (15)
C2—N2—C4—C6	−179.57 (17)	C7—N5—C19—C20	61.98 (19)
N1—C3—C4—N2	0.1 (3)	C15—N5—C19—C20	−56.59 (18)
C5—C3—C4—N2	−179.79 (17)	C11—N5—C19—C20	−177.43 (14)
N1—C3—C4—C6	−179.97 (17)	N5—C19—C20—C21	174.11 (14)
C5—C3—C4—C6	0.2 (3)	C19—C20—C21—C22	178.07 (17)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15*A*···N4^{ii}	0.99	2.59	3.559 (3)	166
C13—H13*A*···S1^{iii}	0.99	2.82	3.748 (2)	157

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