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Aquabis(1,10-phenanthroline-κ^2N,N')-[2,4,6-tris(4-sulfonatophenylamino)-1,3,5-triazin-1-ium-κO]nickel(II) dihydrate

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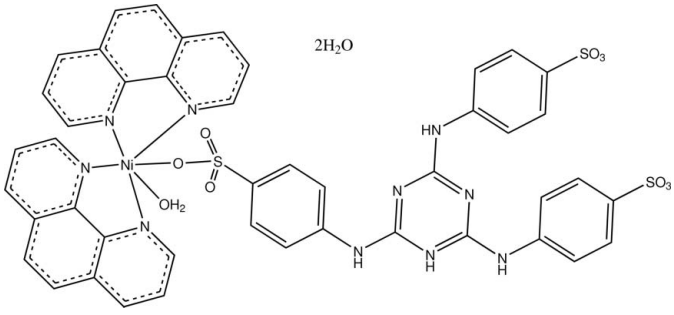
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.047; wR factor = 0.108; data-to-parameter ratio = 14.8.

In the title complex, $[Ni(C_{21}H_{16}N_6O_9S_3)(C_{12}H_8N_2)_2(H_2O)]\cdot 2H_2O$ or $[Ni(HTST)(phen)_2(H_2O)]\cdot 2H_2O$, where H_3TST is 2,4,6-tris(4-sulfophenylamino)-1,3,5-triazine and phen is phenanthroline, the Ni^{II} ion is in a distorted octahedral coordination environment defined by four N atoms from two phen ligands, one O atom from an aqua ligand and one O atom from the SO_3 group of an HTST ligand. In the crystal structure, intermolecular N—H···O and O—H···O hydrogen bonds connect molecules to form a two-dimensional network.

Related literature

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



Experimental

Crystal data

$[Ni(C_{21}H_{16}N_6O_9S_3)(C_{12}H_8N_2)_2(H_2O)]\cdot 2H_2O$
M_r = 1065.74
Triclinic, $P\overline{1}$
a = 8.256 (2) Å
b = 11.684 (3) Å
c = 24.086 (7) Å
α = 76.134 (7)°
β = 84.875 (10)°
γ = 75.718 (6)°
V = 2185.0 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.67 mm^{-1}
T = 293 (2) K
0.25 × 0.10 × 0.08 mm

Data collection

Rigaku Mercury70 diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku Corporation, 2000)
T_{min} = 0.907, T_{max} = 1.000
(expected range = 0.860–0.948)
17176 measured reflections
9893 independent reflections
7634 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.108
S = 1.05
9893 reflections
668 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H2···O5^{i}	0.82 (4)	1.96 (4)	2.756 (3)	165 (4)
O4—H22···O3	0.94 (5)	1.78 (5)	2.691 (3)	162 (4)
O11—H11···O6	0.79 (3)	1.98 (3)	2.768 (4)	177 (3)
O11—H112···O12	0.84 (6)	2.32 (6)	3.045 (4)	144 (6)
O12—H122···O7	0.92 (6)	2.06 (6)	2.944 (4)	160 (5)
N14—H14A···O8^{i}	0.86	2.08	2.887 (3)	156
N15—H15A···O11^{ii}	0.86	2.13	2.974 (3)	166
N16—H16A···O10^{iii}	0.86	2.06	2.864 (3)	155
N13—H13···O10^{iii}	0.84 (3)	2.06 (3)	2.840 (3)	155 (3)
O12—H12···O8^{iv}	0.91 (8)	2.19 (8)	3.035 (4)	155 (7)

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

Data collection: *CrystalClear* (Rigaku Corporation, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* (Bruker, 1998); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2447).

References

Aakeroy, C. B., Desper, J. & Urbina, J. F. (2005). *CrystEngComm*, **7**, 193–201.
Bruker (1998). *XP*. Bruker AXS Inc., Madison, Wisconsin, USA.
Rigaku Corporation (2000). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
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supplementary materials

Acta Cryst. (2007). E**63**, m2119 [**doi:10.1107/S1600536807033223**]

Aquabis(1,10-phenanthroline-κ^2N,N')[2,4,6-tris(4-sulfonatophenylamino)-1,3,5-triazin-1-ium-κO]nickel(II) dihydrate

Y.-F. Yu, Y.-Q. Wei and K.-C. Wu

Comment

In the title complex (Fig. 1), the Ni^{II} atom is six-coordinated by four N atoms from two phen ligands, one O atom from an aqua ligand and one O atom from the SO_3 group of a HTST ligand. The Ni(II)$(phen)_2O_2$ unit of the complex has a *cis* arrangement, with a strong O—H···O H-bond involving the coordinated SO_3^- group and the aqua ligand giving additional stabilization to the coordination environment.

The HTST ligand exists in a negative divalent low-symmetry conformation form (Aakeroy *et al.*, 2005), with two uncoordinated SO_3^- groups, and an H atom transferred to nitrogen atom N13 of the triazine ring. One phen group forms a weak intramolecular π-π stacking interaction (with a ring centroid separation 3.840 (3) Å) with the phenyl ring of the coordinated sulfophenyl group of the HTST ligand.

The two uncoordinated water molecules are hydrogen bonded to two uncoordinated SO_3 groups. In the crystal structure, water molecules, SO_3 groups and N—H groups form a hydrogen-bonded two-dimensional network.

Experimental

The title compound was synthesized by the hydrothermal method from a mixture of $H_3TST{\cdot}7H_2O$ (0.072 g, 0.1 mmol), phen·H_2O (0.059 g, 0.3 mmol), $NiCl_2$ (0.039 g, 0.3 mmol) and water (20.0 mL) in a 25.0 mL Teflon-lined stainless steel reactor. The solution was heated at 433 K for 67 h, and then the reactor was slowly cooled to room temperature to give blue crystals of the title complex.

Refinement

H atoms bonded to O atoms and the H atom bonded to N13 were located in a difference map and refined independently with isotropic displacement parameters. All other H atoms were positioned geometrically and refined using the riding-model approximation with C—H = 0.95–0.99 Å, N—H = 0.86 Å U_{iso}(H) = 1.2 U_{eq} (C,*N*).

Figures

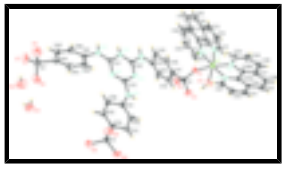


Fig. 1. The molecular structure of the title complex, with atom labels and 50% probability displacement ellipsoids for non-H atoms.

Aquabis(1,10-phenanthroline-κ^2*N*,*N*′)[2,4,6-\ tris(4-sulfonatophenylamino)-1,3,5-triazin-1-ium-κ*O*]nickel(II) dihydrate

Crystal data

$[Ni(C_{21}H_{16}N_6O_9S_3)(C_{12}H_8N_2)_2(H_2O)]\cdot 2H_2O$	$Z = 2$
$M_r = 1065.74$	$F_{000} = 1100$
Triclinic, $P\overline{1}$	$D_x = 1.620$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.256$ (2) Å	Cell parameters from 5038 reflections
$b = 11.684$ (3) Å	$\theta = 2.2$–27.5º
$c = 24.086$ (7) Å	$\mu = 0.67$ mm^{-1}
$\alpha = 76.134$ (7)º	$T = 293$ (2) K
$\beta = 84.875$ (10)º	Prism, blue
$\gamma = 75.718$ (6)º	0.25 × 0.10 × 0.08 mm
$V = 2185.0$ (10) Å^3	

Data collection

Rigaku Mercury70 (2x2 bin mode) diffractometer	9893 independent reflections
Radiation source: fine-focus sealed tube	7634 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.025$
Detector resolution: 14.6306 pixels mm^{-1}	$\theta_{max} = 27.5$º
$T = 293$(2) K	$\theta_{min} = 2.7$º
CCD_Profile_fitting scans	$h = -10\rightarrow10$
Absorption correction: multi-scan (CrystalClear; Rigaku Corporation, 2000)	$k = -15\rightarrow15$
$T_{min} = 0.907$, $T_{max} = 1.000$	$l = -31\rightarrow23$
17176 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.047$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.108$	$w = 1/[\sigma^2(F_o^2) + (0.042P)^2 + 1.2717P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} = 0.001$
9893 reflections	$\Delta\rho_{max} = 0.36$ e Å^{-3}
668 parameters	$\Delta\rho_{min} = -0.37$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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	1.59674 (4)	−0.27469 (3)	0.887559 (13)	0.02613 (9)
S1	1.26211 (8)	−0.37669 (6)	0.88242 (3)	0.03091 (15)
S2	0.60698 (9)	−0.14127 (6)	0.24919 (3)	0.03524 (16)
S3	0.33563 (8)	0.42219 (5)	0.44922 (3)	0.02725 (14)
O1	1.4376 (2)	−0.39381 (15)	0.89659 (7)	0.0308 (4)
O2	1.2008 (3)	−0.48236 (19)	0.90877 (9)	0.0450 (5)
O3	1.1585 (2)	−0.26349 (18)	0.89380 (8)	0.0433 (5)
O4	1.3895 (3)	−0.1304 (2)	0.86597 (11)	0.0467 (6)
H2	1.370 (5)	−0.068 (4)	0.8408 (18)	0.074 (13)*
H22	1.294 (6)	−0.161 (4)	0.8753 (19)	0.096 (16)*
O5	0.7167 (3)	−0.0970 (2)	0.20325 (9)	0.0580 (6)
O6	0.4640 (3)	−0.04557 (19)	0.25793 (10)	0.0567 (6)
O7	0.5617 (3)	−0.24913 (18)	0.24324 (10)	0.0542 (6)
O8	0.4461 (2)	0.47574 (16)	0.40536 (8)	0.0411 (5)
O9	0.2036 (2)	0.38891 (17)	0.42546 (8)	0.0406 (5)
O10	0.2722 (2)	0.49828 (16)	0.48996 (8)	0.0407 (5)
O11	0.1494 (4)	−0.0270 (3)	0.31052 (11)	0.0586 (7)
H11	0.238 (4)	−0.029 (3)	0.2948 (14)	0.034 (9)*
H112	0.137 (8)	−0.097 (6)	0.311 (3)	0.15 (3)*
O12	0.2772 (4)	−0.2985 (3)	0.32023 (16)	0.0765 (8)
H122	0.350 (7)	−0.284 (5)	0.290 (2)	0.12 (2)*
N1	1.6612 (3)	−0.2990 (2)	0.80583 (9)	0.0378 (5)
N2	1.7821 (3)	−0.43427 (18)	0.90611 (9)	0.0298 (5)
N3	1.7329 (3)	−0.14640 (18)	0.88590 (9)	0.0291 (5)
N4	1.5618 (3)	−0.26009 (18)	0.97260 (9)	0.0288 (5)
N11	0.9046 (3)	−0.13966 (17)	0.51045 (8)	0.0257 (4)
N12	1.0119 (3)	−0.18043 (17)	0.60507 (9)	0.0280 (5)
N13	1.1280 (3)	−0.30553 (18)	0.54271 (9)	0.0245 (4)
N14	1.2348 (3)	−0.34576 (18)	0.63237 (9)	0.0287 (5)
H14A	1.3119	−0.3988	0.6200	0.034*
N15	0.8034 (3)	−0.01768 (17)	0.57616 (9)	0.0284 (5)
H15A	0.8079	−0.0143	0.6113	0.034*
N16	1.0174 (3)	−0.28450 (18)	0.45675 (9)	0.0300 (5)

H16A	1.0970	−0.3472	0.4554	0.036*
C10A	1.8304 (3)	−0.4807 (2)	0.85936 (13)	0.0352 (6)
C10B	1.7694 (4)	−0.4083 (3)	0.80575 (13)	0.0415 (7)
C10	1.6035 (5)	−0.2302 (3)	0.75616 (13)	0.0607 (10)
H10B	1.5282	−0.1560	0.7553	0.073*
C11	1.8331 (3)	−0.5018 (2)	0.95668 (13)	0.0392 (7)
H11B	1.8002	−0.4695	0.9888	0.047*
C12	1.9337 (4)	−0.6187 (3)	0.96427 (18)	0.0561 (10)
H12B	1.9650	−0.6636	1.0007	0.067*
C13	1.9848 (4)	−0.6657 (3)	0.9184 (2)	0.0661 (12)
H13B	2.0529	−0.7434	0.9229	0.079*
C14	1.9364 (4)	−0.5983 (3)	0.86341 (19)	0.0576 (10)
C15	1.9817 (5)	−0.6395 (5)	0.8118 (3)	0.0916 (17)
H15B	2.0525	−0.7156	0.8134	0.110*
C16	1.9258 (6)	−0.5726 (6)	0.7618 (3)	0.0989 (19)
H16B	1.9571	−0.6037	0.7293	0.119*
C17	1.8165 (5)	−0.4514 (4)	0.75576 (17)	0.0707 (12)
C18	1.7576 (7)	−0.3771 (6)	0.70484 (19)	0.0961 (18)
H18A	1.7886	−0.4022	0.6708	0.115*
C19	1.6550 (7)	−0.2682 (6)	0.70431 (15)	0.0906 (17)
C20B	1.7261 (3)	−0.1149 (2)	0.93718 (11)	0.0297 (6)
C20A	1.6363 (3)	−0.1765 (2)	0.98362 (11)	0.0288 (5)
C20	1.8099 (4)	−0.0880 (2)	0.84171 (13)	0.0386 (6)
C21	1.4793 (3)	−0.3184 (2)	1.01517 (12)	0.0362 (6)
H21A	1.4274	−0.3753	1.0079	0.043*
C22	1.4662 (4)	−0.2989 (3)	1.07029 (13)	0.0432 (7)
H22A	1.4080	−0.3427	1.0991	0.052*
C23	1.5394 (4)	−0.2150 (3)	1.08170 (13)	0.0440 (7)
H23A	1.5316	−0.2011	1.1184	0.053*
C24	1.6270 (3)	−0.1497 (2)	1.03773 (12)	0.0352 (6)
C25	1.7036 (4)	−0.0566 (3)	1.04464 (14)	0.0455 (8)
H25A	1.6973	−0.0370	1.0801	0.055*
C26	1.7846 (4)	0.0027 (3)	1.00037 (15)	0.0473 (8)
H26A	1.8320	0.0633	1.0060	0.057*
C27	1.8002 (3)	−0.0243 (2)	0.94508 (13)	0.0375 (6)
C28	1.8812 (4)	0.0350 (3)	0.89723 (16)	0.0502 (8)
H28A	1.9317	0.0959	0.9005	0.060*
C29	1.8867 (4)	0.0042 (3)	0.84600 (15)	0.0492 (8)
H29A	1.9405	0.0436	0.8143	0.059*
C31	1.0127 (3)	−0.2398 (2)	0.50303 (10)	0.0234 (5)
C32	1.1225 (3)	−0.2750 (2)	0.59416 (10)	0.0235 (5)
C33	0.9086 (3)	−0.1153 (2)	0.56200 (10)	0.0236 (5)
C41	1.2609 (3)	−0.3620 (2)	0.80735 (11)	0.0301 (6)
C42	1.1728 (4)	−0.2569 (3)	0.77264 (12)	0.0399 (7)
H42A	1.1199	−0.1918	0.7886	0.048*
C43	1.1617 (4)	−0.2467 (2)	0.71471 (12)	0.0396 (7)
H43A	1.1014	−0.1756	0.6920	0.047*
C44	1.2417 (3)	−0.3438 (2)	0.69070 (11)	0.0278 (5)
C45	1.3359 (3)	−0.4479 (2)	0.72549 (11)	0.0342 (6)

H45A	1.3944	−0.5116	0.7094	0.041*
C46	1.3430 (4)	−0.4572 (2)	0.78326 (12)	0.0370 (6)
H46A	1.4035	−0.5280	0.8062	0.044*
C51	0.6872 (3)	0.0800 (2)	0.54398 (11)	0.0258 (5)
C52	0.6232 (3)	0.1770 (2)	0.57027 (11)	0.0306 (6)
H52A	0.6543	0.1719	0.6071	0.037*
C53	0.5141 (3)	0.2803 (2)	0.54208 (11)	0.0293 (6)
H53A	0.4743	0.3452	0.5595	0.035*
C54	0.4643 (3)	0.2870 (2)	0.48802 (10)	0.0252 (5)
C55	0.5232 (3)	0.1893 (2)	0.46230 (11)	0.0293 (5)
H55A	0.4872	0.1932	0.4263	0.035*
C56	0.6350 (3)	0.0860 (2)	0.48978 (11)	0.0275 (5)
H56A	0.6748	0.0214	0.4722	0.033*
C61	0.9109 (3)	−0.2442 (2)	0.40948 (10)	0.0273 (5)
C62	0.8435 (3)	−0.1230 (2)	0.38574 (11)	0.0331 (6)
H62A	0.8617	−0.0627	0.4020	0.040*
C63	0.7488 (4)	−0.0929 (2)	0.33740 (11)	0.0343 (6)
H63A	0.7029	−0.0119	0.3213	0.041*
C64	0.7216 (3)	−0.1817 (2)	0.31291 (10)	0.0278 (5)
C65	0.7886 (3)	−0.3023 (2)	0.33721 (11)	0.0310 (6)
H65A	0.7696	−0.3625	0.3212	0.037*
C66	0.8835 (3)	−0.3333 (2)	0.38514 (11)	0.0318 (6)
H66A	0.9292	−0.4145	0.4012	0.038*
H19A	1.6158	−0.2151	0.6686	0.038*
H20A	1.8137	−0.1094	0.8054	0.038*
H13	1.189 (4)	−0.371 (3)	0.5364 (12)	0.034 (8)*
H12	0.298 (9)	−0.372 (7)	0.345 (3)	0.20 (4)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.03295 (18)	0.02351 (16)	0.02262 (16)	−0.00547 (13)	−0.00518 (13)	−0.00608 (12)
S1	0.0311 (3)	0.0382 (3)	0.0242 (3)	−0.0095 (3)	−0.0061 (3)	−0.0051 (3)
S2	0.0428 (4)	0.0288 (3)	0.0301 (3)	−0.0016 (3)	−0.0131 (3)	−0.0017 (3)
S3	0.0292 (3)	0.0212 (3)	0.0247 (3)	0.0051 (2)	−0.0019 (2)	−0.0034 (2)
O1	0.0326 (10)	0.0302 (9)	0.0310 (10)	−0.0086 (8)	−0.0121 (8)	−0.0043 (8)
O2	0.0475 (12)	0.0554 (12)	0.0368 (11)	−0.0277 (10)	−0.0066 (9)	−0.0012 (10)
O3	0.0402 (11)	0.0496 (12)	0.0368 (11)	0.0017 (9)	−0.0022 (9)	−0.0156 (10)
O4	0.0508 (14)	0.0276 (10)	0.0560 (15)	−0.0020 (10)	−0.0159 (11)	−0.0006 (10)
O5	0.0652 (15)	0.0675 (15)	0.0315 (11)	−0.0143 (12)	−0.0048 (11)	0.0081 (11)
O6	0.0480 (13)	0.0483 (12)	0.0662 (16)	0.0125 (10)	−0.0243 (12)	−0.0149 (11)
O7	0.0777 (16)	0.0367 (11)	0.0521 (13)	−0.0137 (11)	−0.0308 (12)	−0.0067 (10)
O8	0.0426 (11)	0.0287 (9)	0.0397 (11)	0.0014 (8)	0.0069 (9)	0.0028 (8)
O9	0.0360 (11)	0.0431 (11)	0.0383 (11)	−0.0029 (9)	−0.0136 (9)	−0.0026 (9)
O10	0.0486 (12)	0.0286 (9)	0.0346 (11)	0.0142 (9)	−0.0038 (9)	−0.0106 (8)
O11	0.0592 (17)	0.0640 (18)	0.0458 (14)	0.0003 (14)	0.0020 (13)	−0.0159 (13)
O12	0.078 (2)	0.0666 (18)	0.083 (2)	−0.0167 (16)	0.0096 (18)	−0.0187 (17)
N1	0.0549 (15)	0.0425 (13)	0.0242 (11)	−0.0255 (12)	−0.0027 (11)	−0.0080 (10)

N2	0.0263 (11)	0.0285 (10)	0.0353 (12)	−0.0077 (9)	−0.0009 (9)	−0.0075 (9)
N3	0.0305 (11)	0.0268 (10)	0.0306 (11)	−0.0058 (9)	−0.0047 (9)	−0.0070 (9)
N4	0.0285 (11)	0.0298 (10)	0.0271 (11)	−0.0032 (9)	−0.0033 (9)	−0.0076 (9)
N11	0.0288 (11)	0.0223 (9)	0.0227 (10)	0.0024 (8)	−0.0046 (8)	−0.0060 (8)
N12	0.0310 (11)	0.0246 (10)	0.0227 (10)	0.0067 (9)	−0.0052 (9)	−0.0061 (8)
N13	0.0240 (11)	0.0206 (10)	0.0248 (10)	0.0053 (8)	−0.0032 (8)	−0.0074 (8)
N14	0.0295 (11)	0.0271 (10)	0.0242 (11)	0.0070 (9)	−0.0065 (9)	−0.0077 (9)
N15	0.0322 (11)	0.0244 (10)	0.0223 (10)	0.0083 (9)	−0.0047 (9)	−0.0071 (8)
N16	0.0316 (12)	0.0279 (10)	0.0259 (11)	0.0089 (9)	−0.0074 (9)	−0.0116 (9)
C10A	0.0270 (13)	0.0363 (14)	0.0493 (17)	−0.0106 (11)	0.0066 (12)	−0.0225 (13)
C10B	0.0414 (16)	0.0583 (18)	0.0403 (16)	−0.0276 (15)	0.0123 (13)	−0.0291 (15)
C10	0.095 (3)	0.067 (2)	0.0296 (16)	−0.045 (2)	−0.0148 (17)	0.0034 (16)
C11	0.0293 (14)	0.0375 (14)	0.0450 (17)	−0.0078 (12)	−0.0050 (13)	0.0030 (13)
C12	0.0335 (17)	0.0355 (16)	0.090 (3)	−0.0072 (14)	−0.0144 (18)	0.0070 (18)
C13	0.0287 (17)	0.0298 (16)	0.138 (4)	−0.0008 (13)	−0.018 (2)	−0.017 (2)
C14	0.0307 (16)	0.0501 (19)	0.106 (3)	−0.0114 (15)	0.0099 (18)	−0.047 (2)
C15	0.049 (2)	0.099 (4)	0.156 (5)	−0.010 (2)	0.016 (3)	−0.100 (4)
C16	0.065 (3)	0.153 (5)	0.121 (4)	−0.032 (3)	0.037 (3)	−0.119 (4)
C17	0.063 (2)	0.126 (4)	0.054 (2)	−0.049 (2)	0.0264 (19)	−0.061 (2)
C18	0.106 (4)	0.172 (6)	0.050 (3)	−0.079 (4)	0.030 (3)	−0.064 (3)
C19	0.133 (4)	0.145 (5)	0.0194 (16)	−0.091 (4)	−0.006 (2)	−0.003 (2)
C20B	0.0258 (13)	0.0246 (12)	0.0381 (15)	0.0007 (10)	−0.0089 (11)	−0.0098 (11)
C20A	0.0268 (13)	0.0282 (12)	0.0309 (13)	0.0028 (10)	−0.0082 (11)	−0.0127 (11)
C20	0.0382 (16)	0.0348 (14)	0.0406 (16)	−0.0086 (12)	−0.0038 (13)	−0.0034 (12)
C21	0.0353 (15)	0.0388 (14)	0.0341 (15)	−0.0087 (12)	0.0001 (12)	−0.0081 (12)
C22	0.0395 (16)	0.0505 (17)	0.0336 (15)	−0.0022 (14)	0.0011 (13)	−0.0076 (14)
C23	0.0406 (16)	0.0558 (18)	0.0306 (15)	0.0095 (14)	−0.0083 (13)	−0.0187 (14)
C24	0.0296 (14)	0.0381 (14)	0.0367 (15)	0.0082 (11)	−0.0129 (12)	−0.0186 (12)
C25	0.0439 (17)	0.0461 (17)	0.0499 (19)	0.0077 (14)	−0.0203 (15)	−0.0292 (15)
C26	0.0427 (17)	0.0383 (16)	0.068 (2)	0.0005 (14)	−0.0254 (16)	−0.0262 (16)
C27	0.0318 (14)	0.0278 (13)	0.0547 (18)	−0.0023 (11)	−0.0149 (13)	−0.0125 (13)
C28	0.0456 (18)	0.0327 (15)	0.076 (2)	−0.0146 (14)	−0.0168 (17)	−0.0075 (16)
C29	0.0454 (18)	0.0429 (16)	0.057 (2)	−0.0165 (14)	−0.0035 (16)	0.0008 (15)
C31	0.0244 (12)	0.0226 (11)	0.0216 (12)	−0.0024 (9)	−0.0031 (10)	−0.0039 (9)
C32	0.0244 (12)	0.0222 (11)	0.0214 (11)	−0.0014 (9)	−0.0034 (10)	−0.0036 (9)
C33	0.0250 (12)	0.0192 (10)	0.0232 (12)	0.0002 (9)	−0.0027 (10)	−0.0030 (9)
C41	0.0309 (14)	0.0333 (13)	0.0249 (13)	−0.0053 (11)	−0.0089 (11)	−0.0039 (11)
C42	0.0435 (16)	0.0392 (15)	0.0315 (14)	0.0074 (13)	−0.0091 (13)	−0.0125 (12)
C43	0.0480 (17)	0.0321 (14)	0.0298 (14)	0.0111 (12)	−0.0128 (13)	−0.0070 (12)
C44	0.0273 (13)	0.0297 (12)	0.0247 (12)	−0.0023 (10)	−0.0056 (10)	−0.0057 (10)
C45	0.0416 (16)	0.0260 (12)	0.0320 (14)	0.0032 (11)	−0.0116 (12)	−0.0081 (11)
C46	0.0462 (17)	0.0261 (12)	0.0337 (15)	0.0013 (12)	−0.0164 (13)	−0.0020 (11)
C51	0.0229 (12)	0.0210 (11)	0.0284 (13)	0.0031 (9)	−0.0022 (10)	−0.0038 (10)
C52	0.0351 (14)	0.0286 (12)	0.0236 (12)	0.0044 (11)	−0.0046 (11)	−0.0080 (10)
C53	0.0309 (13)	0.0248 (12)	0.0282 (13)	0.0029 (10)	0.0021 (11)	−0.0094 (10)
C54	0.0252 (12)	0.0201 (11)	0.0273 (12)	0.0003 (9)	−0.0015 (10)	−0.0051 (10)
C55	0.0348 (14)	0.0256 (12)	0.0250 (12)	0.0025 (10)	−0.0081 (11)	−0.0077 (10)
C56	0.0308 (13)	0.0210 (11)	0.0295 (13)	0.0020 (10)	−0.0050 (10)	−0.0100 (10)
C61	0.0279 (13)	0.0298 (12)	0.0200 (12)	0.0017 (10)	−0.0019 (10)	−0.0061 (10)

C62	0.0424 (16)	0.0249 (12)	0.0310 (14)	−0.0015 (11)	−0.0061 (12)	−0.0088 (11)
C63	0.0462 (16)	0.0201 (11)	0.0320 (14)	0.0003 (11)	−0.0100 (12)	−0.0022 (10)
C64	0.0307 (13)	0.0262 (12)	0.0237 (12)	−0.0012 (10)	−0.0050 (10)	−0.0041 (10)
C65	0.0378 (15)	0.0268 (12)	0.0298 (13)	−0.0046 (11)	−0.0056 (11)	−0.0104 (11)
C66	0.0374 (15)	0.0232 (12)	0.0301 (14)	0.0031 (11)	−0.0077 (11)	−0.0051 (10)

Geometric parameters (Å, °)

Ni1—N1	2.061 (2)	C14—C15	1.425 (6)
Ni1—N3	2.075 (2)	C15—C16	1.321 (7)
Ni1—N2	2.082 (2)	C15—H15B	0.9300
Ni1—N4	2.085 (2)	C16—C17	1.461 (7)
Ni1—O4	2.087 (2)	C16—H16B	0.9300
Ni1—O1	2.1019 (18)	C17—C18	1.372 (7)
S1—O2	1.435 (2)	C18—C19	1.341 (7)
S1—O3	1.460 (2)	C18—H18A	0.9300
S1—O1	1.4723 (18)	C19—H19A	0.9625
S1—C41	1.776 (3)	C20B—C27	1.402 (4)
S2—O7	1.441 (2)	C20B—C20A	1.431 (4)
S2—O5	1.446 (2)	C20A—C24	1.403 (4)
S2—O6	1.451 (2)	C20—C29	1.405 (4)
S2—C64	1.779 (3)	C20—H20A	0.9604
S3—O9	1.447 (2)	C21—C22	1.391 (4)
S3—O10	1.4574 (19)	C21—H21A	0.9300
S3—O8	1.460 (2)	C22—C23	1.361 (4)
S3—C54	1.772 (2)	C22—H22A	0.9300
O4—H2	0.82 (4)	C23—C24	1.406 (4)
O4—H22	0.94 (5)	C23—H23A	0.9300
O11—H11	0.79 (3)	C24—C25	1.433 (4)
O11—H112	0.84 (6)	C25—C26	1.346 (5)
O12—H122	0.92 (6)	C25—H25A	0.9300
O12—H12	0.91 (8)	C26—C27	1.429 (4)
N1—C10	1.326 (4)	C26—H26A	0.9300
N1—C10B	1.366 (4)	C27—C28	1.402 (4)
N2—C11	1.323 (4)	C28—C29	1.360 (5)
N2—C10A	1.352 (3)	C28—H28A	0.9300
N3—C20	1.322 (3)	C29—H29A	0.9300
N3—C20B	1.364 (3)	C41—C46	1.378 (4)
N4—C21	1.322 (3)	C41—C42	1.383 (4)
N4—C20A	1.361 (3)	C42—C43	1.381 (4)
N11—C31	1.324 (3)	C42—H42A	0.9300
N11—C33	1.343 (3)	C43—C44	1.390 (3)
N12—C32	1.312 (3)	C43—H43A	0.9300
N12—C33	1.357 (3)	C44—C45	1.396 (3)
N13—C32	1.363 (3)	C45—C46	1.375 (4)
N13—C31	1.364 (3)	C45—H45A	0.9300
N13—H13	0.84 (3)	C46—H46A	0.9300
N14—C32	1.341 (3)	C51—C56	1.391 (3)
N14—C44	1.417 (3)	C51—C52	1.397 (3)

N14—H14A	0.8600	C52—C53	1.382 (3)
N15—C33	1.348 (3)	C52—H52A	0.9300
N15—C51	1.412 (3)	C53—C54	1.379 (4)
N15—H15A	0.8600	C53—H53A	0.9300
N16—C31	1.334 (3)	C54—C55	1.392 (3)
N16—C61	1.417 (3)	C55—C56	1.387 (3)
N16—H16A	0.8600	C55—H55A	0.9300
C10A—C10B	1.421 (4)	C56—H56A	0.9300
C10A—C14	1.422 (4)	C61—C66	1.383 (4)
C10B—C17	1.402 (4)	C61—C62	1.387 (3)
C10—C19	1.420 (6)	C62—C63	1.386 (4)
C10—H10B	0.9300	C62—H62A	0.9300
C11—C12	1.392 (4)	C63—C64	1.380 (4)
C11—H11B	0.9300	C63—H63A	0.9300
C12—C13	1.340 (6)	C64—C65	1.383 (3)
C12—H12B	0.9300	C65—C66	1.378 (4)
C13—C14	1.404 (6)	C65—H65A	0.9300
C13—H13B	0.9300	C66—H66A	0.9300
N1—Ni1—N3	97.20 (9)	C10—C19—H19A	119.4
N1—Ni1—N2	80.41 (9)	N3—C20B—C27	122.5 (3)
N3—Ni1—N2	101.02 (8)	N3—C20B—C20A	117.4 (2)
N1—Ni1—N4	173.02 (9)	C27—C20B—C20A	120.1 (2)
N3—Ni1—N4	80.27 (8)	N4—C20A—C24	122.6 (3)
N2—Ni1—N4	93.64 (8)	N4—C20A—C20B	117.2 (2)
N1—Ni1—O4	96.80 (10)	C24—C20A—C20B	120.2 (2)
N3—Ni1—O4	87.21 (9)	N3—C20—C29	122.3 (3)
N2—Ni1—O4	171.55 (9)	N3—C20—H20A	118.9
N4—Ni1—O4	89.60 (9)	C29—C20—H20A	118.9
N1—Ni1—O1	89.19 (8)	N4—C21—C22	123.2 (3)
N3—Ni1—O1	172.66 (8)	N4—C21—H21A	118.4
N2—Ni1—O1	83.55 (8)	C22—C21—H21A	118.4
N4—Ni1—O1	93.79 (8)	C23—C22—C21	119.3 (3)
O4—Ni1—O1	88.46 (9)	C23—C22—H22A	120.3
O2—S1—O3	114.59 (13)	C21—C22—H22A	120.3
O2—S1—O1	110.82 (11)	C22—C23—C24	119.6 (3)
O3—S1—O1	111.61 (11)	C22—C23—H23A	120.2
O2—S1—C41	106.65 (12)	C24—C23—H23A	120.2
O3—S1—C41	106.22 (12)	C20A—C24—C23	117.3 (3)
O1—S1—C41	106.39 (12)	C20A—C24—C25	118.6 (3)
O7—S2—O5	113.16 (15)	C23—C24—C25	124.1 (3)
O7—S2—O6	113.32 (15)	C26—C25—C24	120.8 (3)
O5—S2—O6	111.27 (14)	C26—C25—H25A	119.6
O7—S2—C64	106.78 (12)	C24—C25—H25A	119.6
O5—S2—C64	106.36 (13)	C25—C26—C27	122.2 (3)
O6—S2—C64	105.26 (13)	C25—C26—H26A	118.9
O9—S3—O10	112.51 (12)	C27—C26—H26A	118.9
O9—S3—O8	112.82 (13)	C28—C27—C20B	116.9 (3)
O10—S3—O8	111.72 (12)	C28—C27—C26	124.8 (3)
O9—S3—C54	107.53 (12)	C20B—C27—C26	118.2 (3)

O10—S3—C54	106.41 (11)	C29—C28—C27	120.5 (3)
O8—S3—C54	105.28 (11)	C29—C28—H28A	119.8
S1—O1—Ni1	133.23 (10)	C27—C28—H28A	119.8
Ni1—O4—H2	135 (3)	C28—C29—C20	119.0 (3)
Ni1—O4—H22	108 (3)	C28—C29—H29A	120.5
H2—O4—H22	110 (4)	C20—C29—H29A	120.5
H11—O11—H112	101 (5)	N11—C31—N16	123.1 (2)
H122—O12—H12	119 (6)	N11—C31—N13	122.1 (2)
C10—N1—C10B	118.1 (3)	N16—C31—N13	114.8 (2)
C10—N1—Ni1	129.6 (2)	N12—C32—N14	122.3 (2)
C10B—N1—Ni1	112.07 (18)	N12—C32—N13	120.8 (2)
C11—N2—C10A	118.5 (2)	N14—C32—N13	116.9 (2)
C11—N2—Ni1	128.72 (19)	N11—C33—N15	121.1 (2)
C10A—N2—Ni1	111.64 (18)	N11—C33—N12	126.9 (2)
C20—N3—C20B	118.8 (2)	N15—C33—N12	112.0 (2)
C20—N3—Ni1	128.46 (19)	C46—C41—C42	119.2 (2)
C20B—N3—Ni1	112.54 (17)	C46—C41—S1	120.23 (19)
C21—N4—C20A	117.9 (2)	C42—C41—S1	120.5 (2)
C21—N4—Ni1	129.58 (19)	C43—C42—C41	121.4 (3)
C20A—N4—Ni1	112.49 (17)	C43—C42—H42A	119.3
C31—N11—C33	114.4 (2)	C41—C42—H42A	119.3
C32—N12—C33	116.0 (2)	C42—C43—C44	119.3 (2)
C32—N13—C31	119.45 (19)	C42—C43—H43A	120.3
C32—N13—H13	122 (2)	C44—C43—H43A	120.3
C31—N13—H13	117 (2)	C43—C44—C45	119.1 (2)
C32—N14—C44	127.9 (2)	C43—C44—N14	124.6 (2)
C32—N14—H14A	116.0	C45—C44—N14	116.3 (2)
C44—N14—H14A	116.0	C46—C45—C44	120.7 (2)
C33—N15—C51	131.8 (2)	C46—C45—H45A	119.7
C33—N15—H15A	114.1	C44—C45—H45A	119.7
C51—N15—H15A	114.1	C45—C46—C41	120.3 (2)
C31—N16—C61	129.7 (2)	C45—C46—H46A	119.9
C31—N16—H16A	115.2	C41—C46—H46A	119.9
C61—N16—H16A	115.2	C56—C51—C52	119.5 (2)
N2—C10A—C10B	117.6 (2)	C56—C51—N15	125.4 (2)
N2—C10A—C14	121.6 (3)	C52—C51—N15	115.1 (2)
C10B—C10A—C14	120.9 (3)	C53—C52—C51	120.7 (2)
N1—C10B—C17	122.6 (3)	C53—C52—H52A	119.7
N1—C10B—C10A	117.3 (2)	C51—C52—H52A	119.7
C17—C10B—C10A	120.1 (3)	C54—C53—C52	119.9 (2)
N1—C10—C19	120.8 (4)	C54—C53—H53A	120.1
N1—C10—H10B	119.6	C52—C53—H53A	120.1
C19—C10—H10B	119.6	C53—C54—C55	119.8 (2)
N2—C11—C12	123.3 (3)	C53—C54—S3	120.62 (18)
N2—C11—H11B	118.4	C55—C54—S3	119.48 (19)
C12—C11—H11B	118.4	C56—C55—C54	120.8 (2)
C13—C12—C11	119.1 (3)	C56—C55—H55A	119.6
C13—C12—H12B	120.5	C54—C55—H55A	119.6
C11—C12—H12B	120.5	C55—C56—C51	119.4 (2)

C12—C13—C14	120.5 (3)	C55—C56—H56A	120.3
C12—C13—H13B	119.7	C51—C56—H56A	120.3
C14—C13—H13B	119.7	C66—C61—C62	120.2 (2)
C13—C14—C10A	117.0 (3)	C66—C61—N16	116.1 (2)
C13—C14—C15	125.3 (4)	C62—C61—N16	123.5 (2)
C10A—C14—C15	117.7 (4)	C63—C62—C61	119.0 (2)
C16—C15—C14	121.8 (4)	C63—C62—H62A	120.5
C16—C15—H15B	119.1	C61—C62—H62A	120.5
C14—C15—H15B	119.1	C64—C63—C62	120.9 (2)
C15—C16—C17	122.3 (4)	C64—C63—H63A	119.5
C15—C16—H16B	118.9	C62—C63—H63A	119.5
C17—C16—H16B	118.9	C63—C64—C65	119.5 (2)
C18—C17—C10B	118.0 (4)	C63—C64—S2	120.33 (18)
C18—C17—C16	124.7 (4)	C65—C64—S2	120.11 (19)
C10B—C17—C16	117.3 (4)	C66—C65—C64	120.1 (2)
C19—C18—C17	119.8 (4)	C66—C65—H65A	119.9
C19—C18—H18A	120.1	C64—C65—H65A	119.9
C17—C18—H18A	120.1	C65—C66—C61	120.2 (2)
C18—C19—C10	120.6 (4)	C65—C66—H66A	119.9
C18—C19—H19A	120.0	C61—C66—H66A	119.9
O2—S1—O1—Ni1	−167.03 (14)	C20B—N3—C20—C29	0.8 (4)
O3—S1—O1—Ni1	−38.02 (18)	Ni1—N3—C20—C29	174.7 (2)
C41—S1—O1—Ni1	77.42 (17)	C20A—N4—C21—C22	−0.4 (4)
N1—Ni1—O1—S1	−87.15 (16)	Ni1—N4—C21—C22	−179.9 (2)
N3—Ni1—O1—S1	63.5 (6)	N4—C21—C22—C23	0.8 (4)
N2—Ni1—O1—S1	−167.59 (16)	C21—C22—C23—C24	0.0 (4)
N4—Ni1—O1—S1	99.17 (15)	N4—C20A—C24—C23	1.4 (4)
O4—Ni1—O1—S1	9.67 (16)	C20B—C20A—C24—C23	−178.9 (2)
N3—Ni1—N1—C10	−78.3 (3)	N4—C20A—C24—C25	−177.4 (2)
N2—Ni1—N1—C10	−178.3 (3)	C20B—C20A—C24—C25	2.3 (4)
N4—Ni1—N1—C10	−146.5 (6)	C22—C23—C24—C20A	−1.0 (4)
O4—Ni1—N1—C10	9.8 (3)	C22—C23—C24—C25	177.8 (3)
O1—Ni1—N1—C10	98.1 (3)	C20A—C24—C25—C26	−0.8 (4)
N3—Ni1—N1—C10B	107.66 (19)	C23—C24—C25—C26	−179.6 (3)
N2—Ni1—N1—C10B	7.64 (18)	C24—C25—C26—C27	−0.7 (4)
N4—Ni1—N1—C10B	39.4 (8)	N3—C20B—C27—C28	0.9 (4)
O4—Ni1—N1—C10B	−164.31 (19)	C20A—C20B—C27—C28	−177.9 (2)
O1—Ni1—N1—C10B	−75.95 (19)	N3—C20B—C27—C26	179.4 (2)
N1—Ni1—N2—C11	−176.5 (2)	C20A—C20B—C27—C26	0.7 (4)
N3—Ni1—N2—C11	88.0 (2)	C25—C26—C27—C28	179.3 (3)
N4—Ni1—N2—C11	7.2 (2)	C25—C26—C27—C20B	0.8 (4)
O4—Ni1—N2—C11	−105.2 (7)	C20B—C27—C28—C29	−0.3 (4)
O1—Ni1—N2—C11	−86.2 (2)	C26—C27—C28—C29	−178.7 (3)
N1—Ni1—N2—C10A	−8.92 (17)	C27—C28—C29—C20	0.0 (5)
N3—Ni1—N2—C10A	−104.46 (18)	N3—C20—C29—C28	−0.3 (5)
N4—Ni1—N2—C10A	174.75 (17)	C33—N11—C31—N16	174.0 (2)
O4—Ni1—N2—C10A	62.4 (7)	C33—N11—C31—N13	−5.7 (3)
O1—Ni1—N2—C10A	81.35 (17)	C61—N16—C31—N11	−4.0 (4)
N1—Ni1—N3—C20	9.9 (2)	C61—N16—C31—N13	175.7 (2)

N2—Ni1—N3—C20	91.5 (2)	C32—N13—C31—N11	6.6 (3)
N4—Ni1—N3—C20	−176.7 (2)	C32—N13—C31—N16	−173.1 (2)
O4—Ni1—N3—C20	−86.6 (2)	C33—N12—C32—N14	178.5 (2)
O1—Ni1—N3—C20	−140.5 (5)	C33—N12—C32—N13	−1.4 (3)
N1—Ni1—N3—C20B	−175.90 (17)	C44—N14—C32—N12	9.1 (4)
N2—Ni1—N3—C20B	−94.33 (17)	C44—N14—C32—N13	−170.9 (2)
N4—Ni1—N3—C20B	−2.48 (16)	C31—N13—C32—N12	−2.7 (4)
O4—Ni1—N3—C20B	87.59 (18)	C31—N13—C32—N14	177.4 (2)
O1—Ni1—N3—C20B	33.7 (7)	C31—N11—C33—N15	−178.7 (2)
N1—Ni1—N4—C21	−109.5 (7)	C31—N11—C33—N12	1.3 (4)
N3—Ni1—N4—C21	−178.7 (2)	C51—N15—C33—N11	−6.6 (4)
N2—Ni1—N4—C21	−78.1 (2)	C51—N15—C33—N12	173.4 (2)
O4—Ni1—N4—C21	94.1 (2)	C32—N12—C33—N11	2.2 (4)
O1—Ni1—N4—C21	5.6 (2)	C32—N12—C33—N15	−177.8 (2)
N1—Ni1—N4—C20A	71.0 (7)	O2—S1—C41—C46	−54.7 (3)
N3—Ni1—N4—C20A	1.80 (16)	O3—S1—C41—C46	−177.3 (2)
N2—Ni1—N4—C20A	102.37 (17)	O1—S1—C41—C46	63.7 (2)
O4—Ni1—N4—C20A	−85.44 (17)	O2—S1—C41—C42	122.9 (2)
O1—Ni1—N4—C20A	−173.86 (16)	O3—S1—C41—C42	0.3 (3)
C11—N2—C10A—C10B	177.9 (2)	O1—S1—C41—C42	−118.7 (2)
Ni1—N2—C10A—C10B	8.9 (3)	C46—C41—C42—C43	1.8 (5)
C11—N2—C10A—C14	−1.3 (4)	S1—C41—C42—C43	−175.9 (2)
Ni1—N2—C10A—C14	−170.2 (2)	C41—C42—C43—C44	−0.4 (5)
C10—N1—C10B—C17	−2.2 (4)	C42—C43—C44—C45	−2.0 (4)
Ni1—N1—C10B—C17	172.6 (2)	C42—C43—C44—N14	177.7 (3)
C10—N1—C10B—C10A	179.8 (3)	C32—N14—C44—C43	−19.0 (4)
Ni1—N1—C10B—C10A	−5.3 (3)	C32—N14—C44—C45	160.7 (3)
N2—C10A—C10B—N1	−2.5 (4)	C43—C44—C45—C46	3.2 (4)
C14—C10A—C10B—N1	176.6 (2)	N14—C44—C45—C46	−176.5 (3)
N2—C10A—C10B—C17	179.5 (3)	C44—C45—C46—C41	−1.9 (4)
C14—C10A—C10B—C17	−1.4 (4)	C42—C41—C46—C45	−0.6 (4)
C10B—N1—C10—C19	−1.0 (5)	S1—C41—C46—C45	177.1 (2)
Ni1—N1—C10—C19	−174.8 (3)	C33—N15—C51—C56	11.6 (4)
C10A—N2—C11—C12	−0.3 (4)	C33—N15—C51—C52	−168.0 (3)
Ni1—N2—C11—C12	166.5 (2)	C56—C51—C52—C53	−2.6 (4)
N2—C11—C12—C13	1.2 (5)	N15—C51—C52—C53	177.1 (2)
C11—C12—C13—C14	−0.6 (5)	C51—C52—C53—C54	1.6 (4)
C12—C13—C14—C10A	−0.9 (5)	C52—C53—C54—C55	0.5 (4)
C12—C13—C14—C15	−179.3 (3)	C52—C53—C54—S3	−175.8 (2)
N2—C10A—C14—C13	1.8 (4)	O9—S3—C54—C53	−133.8 (2)
C10B—C10A—C14—C13	−177.3 (3)	O10—S3—C54—C53	−13.0 (2)
N2—C10A—C14—C15	−179.6 (3)	O8—S3—C54—C53	105.7 (2)
C10B—C10A—C14—C15	1.3 (4)	O9—S3—C54—C55	49.9 (2)
C13—C14—C15—C16	177.3 (4)	O10—S3—C54—C55	170.6 (2)
C10A—C14—C15—C16	−1.1 (6)	O8—S3—C54—C55	−70.7 (2)
C14—C15—C16—C17	1.1 (8)	C53—C54—C55—C56	−1.7 (4)
N1—C10B—C17—C18	3.5 (5)	S3—C54—C55—C56	174.7 (2)
C10A—C10B—C17—C18	−178.6 (3)	C54—C55—C56—C51	0.7 (4)
N1—C10B—C17—C16	−176.6 (3)	C52—C51—C56—C55	1.4 (4)

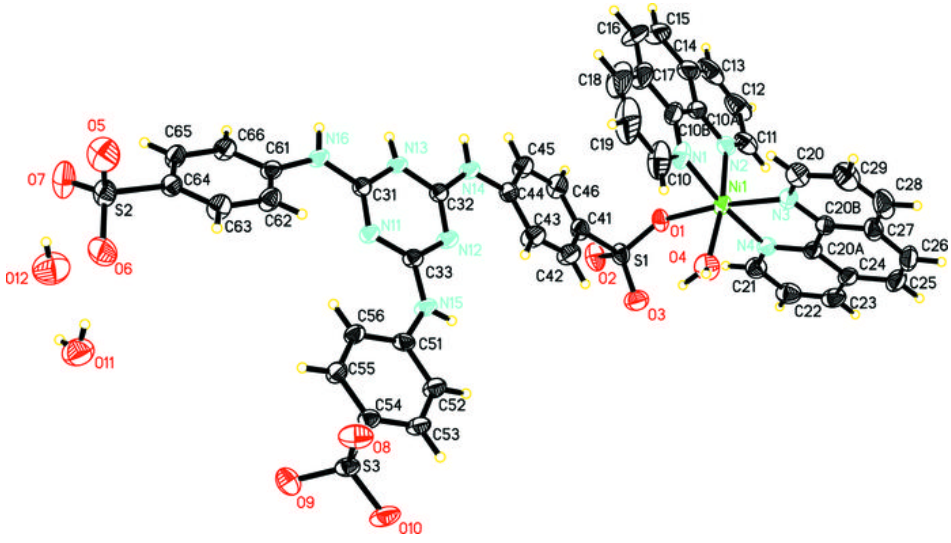
C10A—C10B—C17—C16	1.3 (5)	N15—C51—C56—C55	−178.2 (2)
C15—C16—C17—C18	178.7 (5)	C31—N16—C61—C66	−146.4 (3)
C15—C16—C17—C10B	−1.1 (7)	C31—N16—C61—C62	37.2 (4)
C10B—C17—C18—C19	−1.5 (7)	C66—C61—C62—C63	0.0 (4)
C16—C17—C18—C19	178.7 (4)	N16—C61—C62—C63	176.2 (2)
C17—C18—C19—C10	−1.6 (7)	C61—C62—C63—C64	−0.2 (4)
N1—C10—C19—C18	3.0 (6)	C62—C63—C64—C65	0.5 (4)
C20—N3—C20B—C27	−1.1 (4)	C62—C63—C64—S2	−177.4 (2)
Ni1—N3—C20B—C27	−175.98 (19)	O7—S2—C64—C63	−164.9 (2)
C20—N3—C20B—C20A	177.7 (2)	O5—S2—C64—C63	74.0 (2)
Ni1—N3—C20B—C20A	2.8 (3)	O6—S2—C64—C63	−44.1 (3)
C21—N4—C20A—C24	−0.7 (4)	O7—S2—C64—C65	17.2 (3)
Ni1—N4—C20A—C24	178.86 (19)	O5—S2—C64—C65	−103.9 (2)
C21—N4—C20A—C20B	179.6 (2)	O6—S2—C64—C65	137.9 (2)
Ni1—N4—C20A—C20B	−0.9 (3)	C63—C64—C65—C66	−0.8 (4)
N3—C20B—C20A—N4	−1.3 (3)	S2—C64—C65—C66	177.2 (2)
C27—C20B—C20A—N4	177.5 (2)	C64—C65—C66—C61	0.6 (4)
N3—C20B—C20A—C24	178.9 (2)	C62—C61—C66—C65	−0.2 (4)
C27—C20B—C20A—C24	−2.2 (4)	N16—C61—C66—C65	−176.7 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H2···O5^{i}	0.82 (4)	1.96 (4)	2.756 (3)	165 (4)
O4—H22···O3	0.94 (5)	1.78 (5)	2.691 (3)	162 (4)
O11—H11···O6	0.79 (3)	1.98 (3)	2.768 (4)	177 (3)
O11—H112···O12	0.84 (6)	2.32 (6)	3.045 (4)	144 (6)
O12—H122···O7	0.92 (6)	2.06 (6)	2.944 (4)	160 (5)
N14—H14A···O8^{i}	0.86	2.08	2.887 (3)	156
N15—H15A···O11^{ii}	0.86	2.13	2.974 (3)	166
N16—H16A···O10^{iii}	0.86	2.06	2.864 (3)	155
N13—H13···O10^{iii}	0.84 (3)	2.06 (3)	2.840 (3)	155 (3)
O12—H12···O8^{iv}	0.91 (8)	2.19 (8)	3.035 (4)	155 (7)

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

Fig. 1


C16
C15
C14
C13
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C10A
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C20
C29
C28
C20B
N3
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C20A
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C23
O4
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S1
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C61
C64
C63
C62