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catena-Poly[[nickel(II)-μ_3-1,1-dicyanoethene-2,2-dithiolato-$\kappa^4S,S':N:N'$-bis[(15-crown-5)magnesium(II)]-μ_3-1,1-dicyanoethene-2,2-dithiolato-$\kappa^4N:N':S,S'$] dichloride]

Junli Yang, Chengjuan Li,* Dacheng Li and Daqi Wang

School of Chemistry and Chemical Engineering, Liaocheng University, Liaocheng 252059, People's Republic of China
Correspondence e-mail: dougroup@163.com

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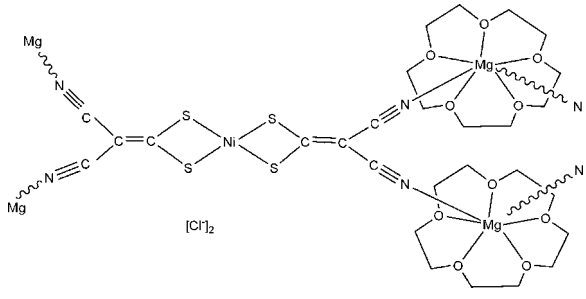
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.026 Å; R factor = 0.064; wR factor = 0.192; data-to-parameter ratio = 8.2.

The reaction of $MgCl_2$, $NiCl_2$, and Na_2(i-mnt) (i-mnt is 1,1-dicyanothene-2,2-dithiolate) with 15-crown-5 (15-C-5) leads to an infinite chain polymer, $\{[NiMg_2(C_4N_2S_2)_2(C_{10}H_{20}O_5)_2]Cl_2\}_n$ or $\{[Mg(15\text{-C-}5)]_2[Ni(i\text{-mnt})_2]Cl_2\}_n$, which consists of two $[Mg(15\text{-C-}5)]^{2+}$ complex cations, one $[Ni(i\text{-mnt})_2]^{2-}$ complex anion and two Cl^- ions per formula unit. In the $[Ni(i\text{-mnt})_2]^{2-}$ complex anion, Ni^{2+} is located on a crystallographic mirror plane with a slightly distorted square-planar coordination by four S atoms. In the $[Mg(15\text{-C-}5)]^{2+}$ complex cations, the Mg and one O atom of the crown lie on mirror planes and the Mg atoms are in sevenfold coordination environments of five O atoms from the crown and two N atoms from two i-mnt anions. The bridging of the two complexes *via* the Mg—N bonds leads to the formation of one-dimensional chains along the *a* axis.

Related literature

For studies on crown ether complexes of alkaline earth metals, see: Junk & Steed (1999). For comparative data on Ni–S bonds, see: Gao *et al.* (2005). For comparative data on Mg–O bonds, see: Chadwick *et al.* (1999).



Experimental

Crystal data

$[NiMg_2(C_4N_2S_2)_2(C_{10}H_{20}O_5)_2]Cl_2$
M_r = 899.11
Orthorhombic, $Cmc2_1$
a = 13.6227 (16) Å
b = 20.591 (3) Å
c = 15.148 (2) Å
V = 4249 (1) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.86 mm^{-1}
T = 298 (2) K
0.41 × 0.32 × 0.30 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.719, T_{max} = 0.783
10632 measured reflections
1979 independent reflections
1651 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.192
S = 1.06
1979 reflections
242 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.92 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}
Absolute structure: Flack (1983), 1979 Friedel pairs
Flack parameter: 0.02 (5)

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SQ2001).

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catena-Poly[[nickel(II)-μ_3-1,1-dicyanoethene-2,2-dithiolato-$\kappa^4S,S':N:N'$-bis[(15-crown-5)magnesium(II)]-μ_3-1,1-dicyanoethene-2,2-dithiolato-$\kappa^4N:N':S,S'$] dichloride]

Junli Yang, Chengjuan Li, Dacheng Li and Daqi Wang

S1. Comment

Crown ethers have gained special attention due to their coordination abilities with not only alkali metal ions, but also alkaline earth ions (Junk & Steed, 1999). In this work, we report the synthesis and structure of a crown ether complex of Mg^{2+} networked with a dithiolate Ni^{II} complex. As shown in Fig. 1, the asymmetric unit of title complex is made up of two half $[Mg(15—C\text{-}5)]^{2+}$ complex cations, one half $[Ni(i\text{-}mnt)_2]^{2-}$ complex anion and two dissociative Cl^- ions on mirror planes. For the two crystallographically independent $[Mg(15—C\text{-}5)]^{2+}$ complex cations, each Mg^{2+} is coordinated by five O atoms of the crown ether with the average Mg–O distance of 2.566 (12) Å, which is far longer than the value in the complex $[Mg(15—C\text{-}5)(SCPh_3)_2]$(2.177 Å) (Chadwick *et al.*, 1999). The additional coordination sites of Mg^{2+} are occupied by two N atoms from cyano groups of the neighboring complex anions $[Ni(i\text{-}mnt)_2]^{2-}$, with the average Mg–N bond length of 2.531 (12) Å. For the complex anion, the Ni^{2+} is coordinated by four S atoms of two $(i\text{-}mnt)^{2-}$ anions in a square planar geometry. The Ni–S bond lengths are in the range of 2.207 (3) to 2.212 (3) Å, which is in perfect agreement with the values (average 2.215 Å) reported in the complex $[Na(N15—C\text{-}5)]_2[Ni(i\text{-}mnt)_2]$ (Gao *et al.*, 2005). Fig. 2 shows that the title complex is assembled into a one-dimensional polymer by the Mg–N bonds between the adjacent $[Mg(15—C\text{-}5)]^{2+}$ complex cations and the $[Ni(i\text{-}mnt)_2]^{2-}$ complex anions along the *a* axis. This motif is similar to what is found in the complex $[Na(N15—C\text{-}5)]_2[Ni(i\text{-}mnt)_2]$, which is also assembled into a one-dimensional stucture by the Na–N bonds between the complex cations and the complex anions. $[Na(N15—C\text{-}5)]_2[Ni(i\text{-}mnt)_2]$ further exhibits a two-dimensional supramolecular structure resulting from π-π stacking interactions between the naphthylene moieties of N15—C-5, which is not observed in the title complex.

S2. Experimental

A solution of $NiCl_2$ (0.2377 g, 0.1 mmol), Na_2(i-mnt) and $MgCl_2$ in methanol (10 ml), was added to a solution of 15-C-5 (0.44 g, 2 mmol) in CH_2Cl_2 (10 ml). The mixture was stirred for 3 hrs at room temperature, and then separated. The underlayer was recrystallized in a mixture of CH_2Cl_2 and ether, and crystals suitable for X-ray diffraction were obtained after two weeks (m.p. 471–473 K). Analysis calc. for $C_{28}H_{40}Cl_2Mg_2N_4O_{10}S_4$: C 37.37, H 4.49, N 6.23%; found: C 37.29, H 4.40, N 6.32%.

S3. Refinement

All H atoms were placed in geometrically idealized positions (C–H 0.97 Å) and treated as riding on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C). 1979 Friedel pairs were used to determine the Flack parameter.

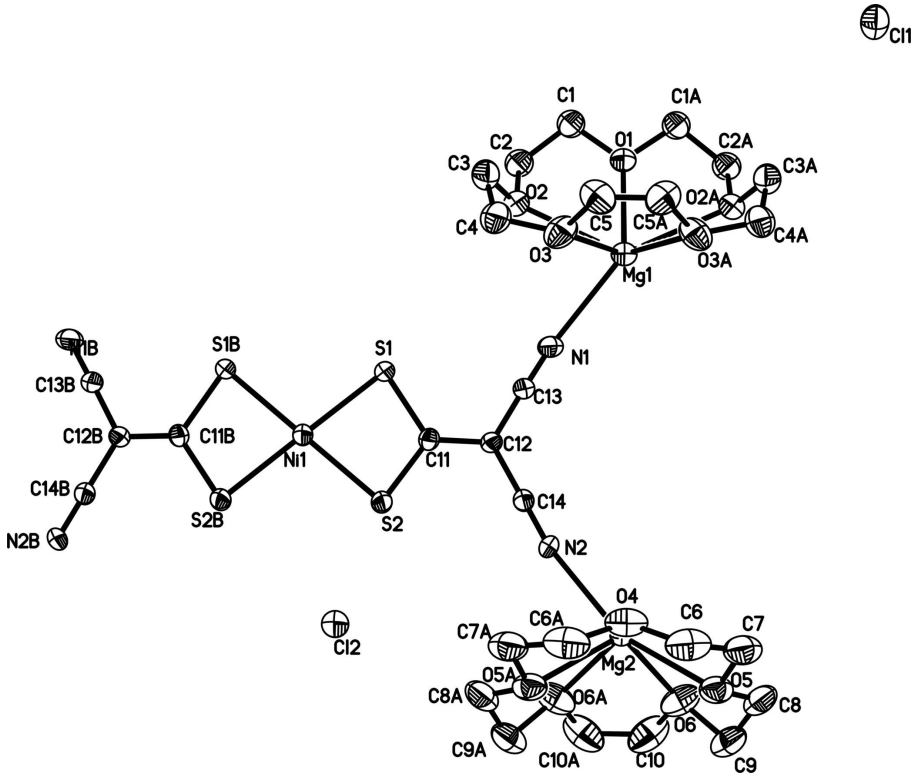

Figure 1

The molecular structure of (I), with atom labels and 20% probability displacement ellipsoids for non-H atoms. Symmetry codes: (A) 1 - *x*, +*y*, +*z*; (B) -*x*, +*y*, +*z*.

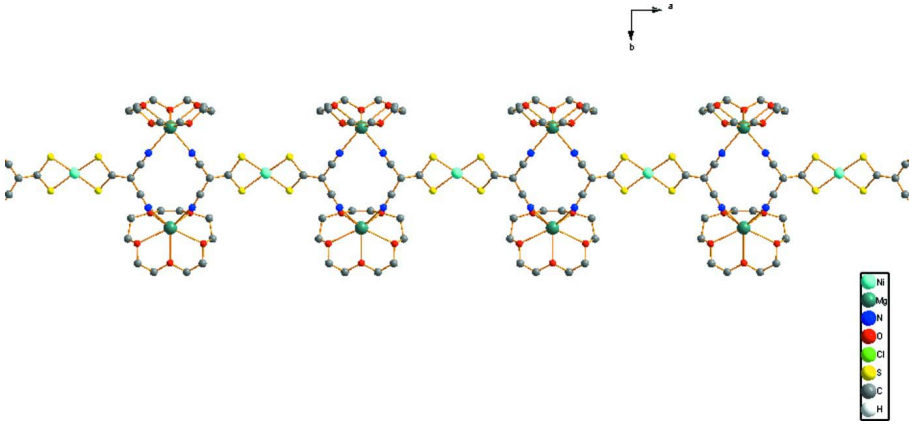

Figure 2

One-dimensional chain-like structure of the title complex (Cl^- ions are omitted).

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Crystal data

$[NiMg_2(C_4N_2S_2)_2(C_{10}H_{20}O_5)_2]Cl_2$
M_r = 899.11

Orthorhombic, *Cmc*2$_1$
Hall symbol: C 2c -2

a = 13.6227 (16) Å
b = 20.591 (3) Å
c = 15.148 (2) Å
V = 4249 (1) Å^3
Z = 4
F(000) = 1864
D_x = 1.406 Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4296 reflections
θ = 2.2–24.9°
μ = 0.86 mm^{-1}
T = 298 K
Block, brown
0.41 × 0.32 × 0.30 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.719, T_{max} = 0.783

10632 measured reflections
1979 independent reflections
1651 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 25.0°, θ_{min} = 2.4°
h = −16→16
k = −24→23
l = −9→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.192
S = 1.06
1979 reflections
242 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.1309P)^2 + 12.7693P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.92 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}
Absolute structure: Flack (1983)
Absolute structure parameter: 0.02 (5)

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	0.0000	0.12793 (7)	0.9803 (2)	0.0492 (4)
Mg1	0.5000	0.3176 (3)	1.0866 (4)	0.0713 (14)
Mg2	0.5000	−0.0308 (2)	0.8135 (3)	0.0565 (11)
N1	0.3850 (8)	0.2476 (5)	0.9910 (9)	0.093 (4)
N2	0.3863 (6)	0.0587 (5)	0.8547 (8)	0.074 (3)
O1	0.5000	0.4399 (6)	1.1122 (9)	0.084 (3)
O2	0.3268 (7)	0.3721 (4)	1.1116 (7)	0.084 (2)
O3	0.3963 (10)	0.2655 (6)	1.2030 (8)	0.112 (4)

O4	0.5000	−0.0908 (6)	0.9581 (9)	0.109 (5)
O5	0.6412 (9)	−0.1054 (5)	0.8323 (8)	0.103 (3)
O6	0.5988 (12)	−0.0446 (7)	0.6826 (9)	0.131 (4)
Cl1	0.0000	0.9064 (4)	0.8312 (9)	0.159 (4)
Cl2	0.0000	0.2859 (4)	0.2265 (8)	0.149 (3)
S1	0.12480 (17)	0.18894 (12)	1.02320 (19)	0.0571 (6)
S2	0.12522 (16)	0.07215 (11)	0.9274 (2)	0.0564 (6)
C1	0.4140 (11)	0.4707 (7)	1.1444 (12)	0.095 (4)
H1A	0.4158	0.5167	1.1309	0.114*
H1B	0.4095	0.4655	1.2079	0.114*
C2	0.3302 (12)	0.4407 (6)	1.1020 (12)	0.098 (4)
H2A	0.2706	0.4591	1.1265	0.118*
H2B	0.3316	0.4512	1.0395	0.118*
C3	0.2781 (12)	0.3557 (9)	1.1909 (12)	0.100 (4)
H3A	0.2084	0.3647	1.1863	0.120*
H3B	0.3047	0.3803	1.2401	0.120*
C4	0.2959 (14)	0.2843 (9)	1.2035 (13)	0.108 (5)
H4A	0.2670	0.2712	1.2592	0.129*
H4B	0.2620	0.2609	1.1569	0.129*
C5	0.4508 (14)	0.2588 (10)	1.2820 (11)	0.116 (6)
H5A	0.4301	0.2936	1.3210	0.140*
H5B	0.4301	0.2185	1.3093	0.140*
C6	0.589 (2)	−0.1249 (9)	0.9749 (16)	0.132 (7)
H6A	0.5784	−0.1707	0.9635	0.159*
H6B	0.6055	−0.1202	1.0368	0.159*
C7	0.674 (2)	−0.1019 (10)	0.9200 (15)	0.130 (7)
H7A	0.6922	−0.0577	0.9353	0.156*
H7B	0.7311	−0.1297	0.9287	0.156*
C8	0.7145 (16)	−0.0869 (10)	0.7714 (16)	0.123 (6)
H8A	0.7715	−0.1148	0.7775	0.147*
H8B	0.7347	−0.0425	0.7823	0.147*
C9	0.6722 (17)	−0.0931 (10)	0.6793 (15)	0.127 (7)
H9A	0.7209	−0.0838	0.6343	0.152*
H9B	0.6445	−0.1358	0.6691	0.152*
C10	0.552 (2)	−0.0474 (13)	0.600 (2)	0.172 (11)
H10A	0.5743	−0.0863	0.5698	0.206*
H10B	0.5743	−0.0105	0.5652	0.206*
C11	0.1961 (6)	0.1356 (4)	0.9620 (6)	0.051 (2)
C12	0.2935 (7)	0.1459 (4)	0.9403 (7)	0.0521 (19)
C13	0.3435 (7)	0.2023 (5)	0.9693 (8)	0.061 (2)
C14	0.3456 (7)	0.0975 (5)	0.8923 (8)	0.057 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0437 (7)	0.0506 (8)	0.0532 (8)	0.000	0.000	−0.0009 (7)
Mg1	0.077 (3)	0.067 (3)	0.069 (3)	0.000	0.000	−0.006 (3)
Mg2	0.057 (2)	0.058 (2)	0.055 (2)	0.000	0.000	−0.009 (2)

N1	0.075 (6)	0.090 (7)	0.116 (9)	−0.019 (5)	0.025 (6)	−0.051 (7)
N2	0.044 (4)	0.075 (6)	0.104 (7)	0.008 (4)	0.006 (5)	−0.033 (6)
O1	0.080 (8)	0.071 (7)	0.101 (9)	0.000	0.000	−0.023 (6)
O2	0.078 (5)	0.086 (5)	0.089 (6)	0.005 (4)	0.003 (5)	−0.012 (5)
O3	0.121 (9)	0.138 (9)	0.077 (6)	0.016 (7)	0.026 (6)	0.007 (6)
O4	0.185 (16)	0.072 (7)	0.069 (8)	0.000	0.000	0.007 (6)
O5	0.126 (9)	0.080 (6)	0.103 (8)	0.020 (6)	−0.031 (7)	−0.013 (6)
O6	0.173 (12)	0.117 (9)	0.103 (9)	0.033 (9)	0.043 (9)	0.004 (7)
Cl1	0.130 (6)	0.122 (5)	0.225 (11)	0.000	0.000	0.018 (7)
Cl2	0.115 (5)	0.136 (5)	0.197 (9)	0.000	0.000	0.046 (6)
S1	0.0443 (12)	0.0618 (13)	0.0652 (14)	0.0027 (9)	0.0003 (11)	−0.0202 (12)
S2	0.0471 (12)	0.0464 (11)	0.0757 (15)	0.0005 (8)	0.0012 (12)	−0.0051 (11)
C1	0.092 (9)	0.084 (8)	0.108 (11)	0.010 (7)	−0.009 (9)	−0.006 (8)
C2	0.096 (10)	0.081 (8)	0.117 (11)	0.016 (7)	−0.011 (9)	−0.009 (8)
C3	0.085 (9)	0.116 (12)	0.100 (11)	−0.005 (8)	0.004 (8)	−0.006 (9)
C4	0.103 (11)	0.120 (12)	0.101 (11)	−0.014 (9)	0.026 (9)	−0.002 (10)
C5	0.132 (13)	0.136 (14)	0.081 (9)	−0.036 (10)	0.006 (9)	0.012 (9)
C6	0.21 (2)	0.098 (11)	0.085 (9)	0.031 (14)	−0.032 (16)	0.003 (9)
C7	0.161 (19)	0.104 (12)	0.126 (16)	0.037 (12)	−0.043 (15)	−0.029 (12)
C8	0.121 (15)	0.108 (12)	0.140 (16)	0.038 (11)	0.015 (14)	−0.022 (12)
C9	0.138 (16)	0.110 (13)	0.132 (16)	0.022 (12)	0.044 (14)	−0.013 (11)
C10	0.20 (3)	0.18 (2)	0.135 (18)	0.064 (19)	0.041 (18)	−0.006 (17)
C11	0.046 (4)	0.052 (4)	0.055 (6)	0.007 (4)	−0.005 (4)	0.001 (4)
C12	0.052 (5)	0.049 (4)	0.055 (5)	0.006 (4)	−0.002 (4)	−0.005 (4)
C13	0.053 (5)	0.062 (5)	0.066 (6)	−0.002 (4)	0.004 (5)	−0.017 (5)
C14	0.048 (5)	0.052 (5)	0.072 (6)	0.000 (4)	−0.003 (5)	−0.006 (5)

Geometric parameters (Å, º)

Ni1—S2^{i}	2.207 (3)	O6—C10	1.41 (3)
Ni1—S2	2.207 (3)	O6—C9	1.41 (2)
Ni1—S1	2.212 (3)	S1—C11	1.734 (9)
Ni1—S1^{i}	2.212 (3)	S2—C11	1.708 (9)
Mg1—O3	2.502 (13)	C1—C2	1.45 (2)
Mg1—O3^{ii}	2.502 (13)	C1—H1A	0.9700
Mg1—O1	2.548 (13)	C1—H1B	0.9700
Mg1—N1	2.575 (12)	C2—H2A	0.9700
Mg1—N1^{ii}	2.575 (12)	C2—H2B	0.9700
Mg1—O2^{ii}	2.640 (10)	C3—C4	1.50 (2)
Mg1—O2	2.640 (10)	C3—H3A	0.9700
Mg2—O6^{ii}	2.414 (12)	C3—H3B	0.9700
Mg2—O6	2.414 (12)	C4—H4A	0.9700
Mg2—O5^{ii}	2.478 (11)	C4—H4B	0.9700
Mg2—O5	2.478 (11)	C5—H5A	0.9700
Mg2—N2^{ii}	2.487 (10)	C5—H5B	0.9700
Mg2—N2	2.487 (9)	C6—C7	1.51 (3)
Mg2—O4	2.514 (14)	C6—H6A	0.9700
N1—C13	1.140 (13)	C6—H6B	0.9700

N2—C14	1.128 (13)	C7—H7A	0.9700
O1—C1^{ii}	1.418 (16)	C7—H7B	0.9700
O1—C1	1.418 (16)	C8—C9	1.51 (3)
O2—C3	1.41 (2)	C8—H8A	0.9700
O2—C2	1.420 (15)	C8—H8B	0.9700
O3—C5	1.41 (2)	C9—H9A	0.9700
O3—C4	1.42 (2)	C9—H9B	0.9700
O4—C6	1.42 (2)	C10—H10A	0.9700
O4—C6^{ii}	1.42 (2)	C10—H10B	0.9700
O5—C7	1.40 (2)	C11—C12	1.383 (13)
O5—C8	1.41 (2)		

S2^{i}—Ni1—S2	101.24 (16)	C11—S2—Ni1	85.8 (3)
S2^{i}—Ni1—S1	175.2 (2)	O1—C1—C2	108.0 (12)
S2—Ni1—S1	78.94 (8)	O1—C1—H1A	110.1
S2^{i}—Ni1—S1^{i}	78.94 (8)	C2—C1—H1A	110.1
S2—Ni1—S1^{i}	175.2 (2)	O1—C1—H1B	110.1
S1—Ni1—S1^{i}	100.48 (15)	C2—C1—H1B	110.1
O3—Mg1—O3^{ii}	68.8 (6)	H1A—C1—H1B	108.4
O3—Mg1—O1	108.5 (4)	O2—C2—C1	113.8 (12)
O3^{ii}—Mg1—O1	108.5 (4)	O2—C2—H2A	108.8
O3—Mg1—N1	79.2 (4)	C1—C2—H2A	108.8
O3^{ii}—Mg1—N1	120.0 (5)	O2—C2—H2B	108.8
O1—Mg1—N1	129.7 (4)	C1—C2—H2B	108.8
O3—Mg1—N1^{ii}	120.0 (5)	H2A—C2—H2B	107.7
O3^{ii}—Mg1—N1^{ii}	79.2 (4)	O2—C3—C4	105.4 (13)
O1—Mg1—N1^{ii}	129.7 (4)	O2—C3—H3A	110.7
N1—Mg1—N1^{ii}	74.9 (5)	C4—C3—H3A	110.7
O3—Mg1—O2^{ii}	125.9 (4)	O2—C3—H3B	110.7
O3^{ii}—Mg1—O2^{ii}	64.9 (4)	C4—C3—H3B	110.7
O1—Mg1—O2^{ii}	63.8 (2)	H3A—C3—H3B	108.8
N1—Mg1—O2^{ii}	149.6 (4)	O3—C4—C3	114.9 (14)
N1^{ii}—Mg1—O2^{ii}	77.0 (3)	O3—C4—H4A	108.5
O3—Mg1—O2	64.9 (4)	C3—C4—H4A	108.5
O3^{ii}—Mg1—O2	125.9 (4)	O3—C4—H4B	108.5
O1—Mg1—O2	63.8 (2)	C3—C4—H4B	108.5
N1—Mg1—O2	77.0 (3)	H4A—C4—H4B	107.5
N1^{ii}—Mg1—O2	149.6 (4)	C5^{ii}—C5—O3	121.6 (8)
O2^{ii}—Mg1—O2	126.7 (4)	C5^{ii}—C5—H5A	106.9
O6^{ii}—Mg2—O6	67.8 (9)	O3—C5—H5A	106.9
O6^{ii}—Mg2—O5^{ii}	65.7 (5)	C5^{ii}—C5—H5B	106.9
O6—Mg2—O5^{ii}	117.0 (5)	O3—C5—H5B	106.9
O6^{ii}—Mg2—O5	117.0 (5)	H5A—C5—H5B	106.7
O6—Mg2—O5	65.7 (5)	O4—C6—C7	113.9 (16)
O5^{ii}—Mg2—O5	101.9 (6)	O4—C6—H6A	108.8
O6^{ii}—Mg2—N2^{ii}	129.8 (5)	C7—C6—H6A	108.8
O6—Mg2—N2^{ii}	86.9 (5)	O4—C6—H6B	108.8
O5^{ii}—Mg2—N2^{ii}	156.1 (4)	C7—C6—H6B	108.8

O5—Mg2—N2^{ii}	87.0 (3)	H6A—C6—H6B	107.7
O6^{ii}—Mg2—N2	86.9 (5)	O5—C7—C6	104.8 (19)
O6—Mg2—N2	129.8 (5)	O5—C7—H7A	110.8
O5^{ii}—Mg2—N2	87.0 (3)	C6—C7—H7A	110.8
O5—Mg2—N2	156.1 (4)	O5—C7—H7B	110.8
N2^{ii}—Mg2—N2	77.0 (4)	C6—C7—H7B	110.8
O6^{ii}—Mg2—O4	131.1 (4)	H7A—C7—H7B	108.9
O6—Mg2—O4	131.1 (4)	O5—C8—C9	108.1 (17)
O5^{ii}—Mg2—O4	66.1 (4)	O5—C8—H8A	110.1
O5—Mg2—O4	66.1 (4)	C9—C8—H8A	110.1
N2^{ii}—Mg2—O4	98.4 (4)	O5—C8—H8B	110.1
N2—Mg2—O4	98.4 (4)	C9—C8—H8B	110.1
C13—N1—Mg1	157.3 (12)	H8A—C8—H8B	108.4
C14—N2—Mg2	163.5 (10)	O6—C9—C8	100.3 (15)
C1^{ii}—O1—C1	111.5 (14)	O6—C9—H9A	111.7
C1^{ii}—O1—Mg1	119.6 (7)	C8—C9—H9A	111.7
C1—O1—Mg1	119.6 (8)	O6—C9—H9B	111.7
C3—O2—C2	109.9 (13)	C8—C9—H9B	111.7
C3—O2—Mg1	116.1 (9)	H9A—C9—H9B	109.5
C2—O2—Mg1	112.2 (9)	O6—C10—C10^{ii}	116.9 (12)
C5—O3—C4	121.8 (13)	O6—C10—H10A	108.1
C5—O3—Mg1	110.0 (10)	C10^{ii}—C10—H10A	108.1
C4—O3—Mg1	115.4 (10)	O6—C10—H10B	108.1
C6—O4—C6^{ii}	117 (2)	C10^{ii}—C10—H10B	108.1
C6—O4—Mg2	113.4 (13)	H10A—C10—H10B	107.3
C6^{ii}—O4—Mg2	113.4 (13)	C12—C11—S2	125.9 (7)
C7—O5—C8	112.1 (18)	C12—C11—S1	124.6 (7)
C7—O5—Mg2	109.1 (11)	S2—C11—S1	109.4 (5)
C8—O5—Mg2	107.9 (10)	C11—C12—C13	120.9 (8)
C10—O6—C9	105.1 (16)	C11—C12—C14	119.5 (8)
C10—O6—Mg2	119.0 (14)	C13—C12—C14	119.5 (8)
C9—O6—Mg2	120.5 (12)	N1—C13—C12	178.5 (12)
C11—S1—Ni1	85.1 (3)	N2—C14—C12	179.3 (13)

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