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Poly[[bis(18-crown-6)bis(μ_3-1,1-dicyanoethylene-2,2-dithiolato)dipotassium(I)-nickelate(II)] 1,2-dichloroethane solvate]

Shi-Zhou Fu, Da-Qi Wang* and Jian-Ming Dou

College of Chemistry and Chemical Engineering, Liaocheng University, Shandong 252059, People's Republic of China
Correspondence e-mail: wdq@lcu.edu.cn

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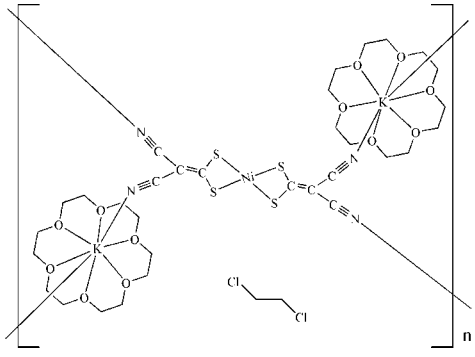
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.043; wR factor = 0.128; data-to-parameter ratio = 18.6.

The title complex, $[K_2Ni(C_4N_2S_2)_2(C_{12}H_{24}O_6)_2]\cdot C_2H_4Cl_2$, consists of two symmetry-equivalent $[K(18C6)]^+$ complex cations (18C6 = 18-crown-6), one centrosymmetric $[Ni(i\text{-}mnt)_2]^{2-}$ complex anion (i-mnt = 1,1-dicyanoethylene-2,2-dithiolate), and a $ClCH_2CH_2Cl$ solvent molecule that also lies on an inversion center. The $[K(18C6)]^+$ cations and $[Ni(i\text{-}mnt)_2]^{2-}$ complex anions form a two-dimensional network through K···N interactions.

Related literature

For related literature, see: Chen & Suslick (1993); Long *et al.* (1998); Nakamura *et al.* (1998).



Experimental

Crystal data

$[K_2Ni(C_4N_2S_2)_2(C_{12}H_{24}O_6)_2]\cdot C_2H_4Cl_2$
M_r = 1044.85
Monoclinic, $P2_1/c$
a = 8.271 (1) Å
b = 13.067 (2) Å
c = 22.207 (2) Å
β = 90.140 (2)°
V = 2400.1 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.92 mm^{-1}
T = 298 (2) K
0.40 × 0.32 × 0.31 mm

Data collection

Siemens SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.710, T_{max} = 0.763
13861 measured reflections
4882 independent reflections
2717 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.128
S = 1.01
4882 reflections
262 parameters
3 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.77 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—S2	2.2101 (10)	K1—O2	2.806 (3)
Ni1—S1	2.2170 (10)	K1—O3	2.828 (3)
K1—O6	2.727 (3)	K1—N2^{i}	2.879 (4)
K1—O1	2.793 (3)	K1—N1	3.021 (3)
K1—O4	2.794 (3)		
S2—Ni1—S1	78.29 (4)		

Symmetry code: (i) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); 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: CF2109).

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supplementary materials

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Poly[[bis(18-crown-6)bis(μ_3-1,1-dicyanoethylene-2,2-dithiolato)dipotassium(I)nickelate(II)] 1,2-dichloroethane solvate]

S.-Z. Fu, D.-Q. Wang and J.-M. Dou

Comment

In recent years, metal coordination complexes with one-dimensional polymeric structures have attracted interest owing to their important applications as materials with unusual properties (Chen &Suslick, 1993). The complexes formed by crown ethers, alkali metal cations, and transition metal bis(dithiolate) anions, in which the bis(dithiolate) ligands include i-mnt (Long *et al.*, 1998) have attracted widespread interest due to their unusual crystal structures and nusual electrical, magnetic and optical properties (Nakamura *et al.*, 1998). The title complex consists of two $[K(18\ C6)]^+$ complex cations, one centrosymmetric $[Ni(i\text{-}mnt)_2]^{2-}$ complex anion, and a solvent molecule. The Ni atom is located on an inversion center and does not bond directly to the O atoms of the crown ether. It is coordinated by four S atoms from two i-mnt ligands. The NiS_4 group is square planar. In the complex cation $[K(18\ C6)]^+$, the potassium ion lies within the crown ether cavity, 0.2038Å out of the plane formed by the six ether oxygen atoms. The K^+ ion is also coordinated by two N atoms from i-mnt ligands of different $[Ni(i\text{-}mnt)_2]^{2-}$ complex anions. Thus the $[K(18\ C6)]^+$ cations and $[Ni(i\text{-}mnt)_2]^{2-}$ complex anions form a two-dimensional network bridged by K—N interactions. The solvent molecule also lies on an inversion center.

Experimental

To a solution of 18-crown-6 (2.0 mmol) in 1,2-dichloroethane (10.0 ml) was added 5 ml of 1,2-dichloroethane containing $NiCl_2$ (0.5 mmol) and K_2(i-mnt) (1 mmol). The reaction mixture was stirred for 2 h at room temperature and then filtered. The precipitate was dissolved in 4:1 diethyl ether/1,2-dichloroethane. Colorless single crystals were obtained by slowly evaporating the solution. Elemental analysis found: H 5.02, C 39.08, N 5.36%; calculated for $C_{34}H_{52}Cl_2K_2N_4O_{12}S_4Ni$: H 5.23, C 38.93, N 5.12%.

Refinement

All H atoms were positioned geometrically and treated as riding on their parent atoms, with 0.97Å and the U_{iso}(H) values were set at $1.2U_{eq}$(C) for C-bound H atoms..

Figures

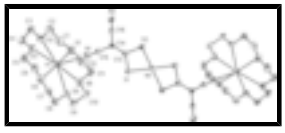


Fig. 1. A segment of the polymeric structure of the title complex, showing 30% probability displacement ellipsoids and the atom-numbering scheme. H atoms and the solvent molecule have been omitted for clarity. [Symmetry code for unlabeled atoms: $1-x$, $1-y$, $1-z$.]

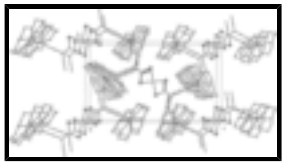


Fig. 2. Crystal packing of the title complex. H atoms and solvent molecules have been omitted.

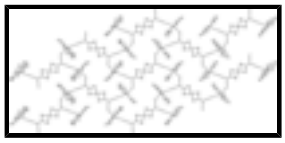


Fig. 3. Two-dimensional sheet network of the title complex. H atoms and solvent molecules have been omitted.

Poly[[bis(18-crown-6)bis(μ$_3$-1,1-dicyanoethylene-2,2-\ dithiolato)dipotassium(I)nickelate(II)] 1,2-dichloroethane solvate]

Crystal data

$[K_2Ni(C_4N_2S_2)_2(C_{12}H_{24}O_6)_2]\cdot C_2H_4Cl_2$	F_{000} = 1088
M_r = 1044.85	D_x = 1.446 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 2404 reflections
a = 8.271 (1) Å	θ = 2.4–20.9º
b = 13.067 (2) Å	μ = 0.92 mm^{-1}
c = 22.207 (2) Å	T = 298 (2) K
β = 90.140 (2)º	Block, colourless
V = 2400.1 (5) Å^3	0.40 × 0.32 × 0.31 mm
Z = 2	

Data collection

Siemens SMART CCD diffractometer	4882 independent reflections
Radiation source: fine-focus sealed tube	2717 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.041
T = 298(2) K	θ_{max} = 26.4º
φ and ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −10→10
T_{min} = 0.710, T_{max} = 0.763	k = −11→16
13861 measured reflections	l = −27→26

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.044	H-atom parameters constrained
$wR(F^2)$ = 0.128	$w = 1/[\sigma^2(F_o^2) + (0.0507P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

S = 1.01	$(\Delta/\sigma)_{max} < 0.001$
4882 reflections	$\Delta\rho_{max} = 0.59$ e Å^{-3}
262 parameters	$\Delta\rho_{min} = -0.77$ e Å^{-3}
3 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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	0.5000	0.5000	0.5000	0.0446 (2)
K1	−0.04263 (11)	0.51950 (6)	0.17024 (4)	0.0524 (2)
Cl1	0.11657 (19)	0.41379 (12)	0.56953 (7)	0.1072 (5)
N1	0.1579 (4)	0.6009 (2)	0.27356 (14)	0.0524 (2)
N2	0.2288 (5)	0.8652 (3)	0.39120 (16)	0.0765 (12)
O1	−0.2843 (4)	0.4976 (2)	0.25695 (13)	0.0724 (9)
O2	−0.3427 (4)	0.6163 (2)	0.15473 (14)	0.0680 (8)
O3	−0.0790 (4)	0.6762 (2)	0.08341 (13)	0.0680 (8)
O4	0.1728 (4)	0.5284 (2)	0.07367 (12)	0.0675 (8)
O5	0.2242 (3)	0.3857 (2)	0.16313 (12)	0.0603 (8)
O6	−0.0334 (4)	0.3540 (2)	0.24499 (12)	0.0645 (8)
S1	0.38775 (13)	0.48585 (7)	0.40962 (4)	0.0531 (3)
S2	0.43037 (13)	0.66007 (7)	0.48093 (4)	0.0513 (3)
C1	−0.4432 (6)	0.5184 (4)	0.2352 (2)	0.0839 (15)
H1A	−0.5184	0.5191	0.2687	0.101*
H1B	−0.4763	0.4648	0.2076	0.101*
C2	−0.4478 (6)	0.6182 (4)	0.2041 (2)	0.0783 (14)
H2A	−0.5570	0.6324	0.1905	0.094*
H2B	−0.4155	0.6720	0.2318	0.094*
C3	−0.3468 (6)	0.7057 (4)	0.1196 (2)	0.0769 (14)
H3A	−0.3095	0.7636	0.1432	0.092*
H3B	−0.4568	0.7194	0.1066	0.092*
C4	−0.2412 (6)	0.6917 (4)	0.0663 (2)	0.0791 (14)
H4A	−0.2785	0.6332	0.0432	0.095*
H4B	−0.2484	0.7517	0.0408	0.095*
C5	0.0254 (6)	0.6647 (4)	0.0331 (2)	0.0811 (15)

H5A	0.0360	0.7298	0.0125	0.097*
H5B	−0.0212	0.6159	0.0050	0.097*
C6	0.1863 (6)	0.6287 (4)	0.0522 (2)	0.0791 (14)
H6A	0.2604	0.6308	0.0185	0.095*
H6B	0.2282	0.6729	0.0837	0.095*
C7	0.3235 (5)	0.4777 (4)	0.08011 (19)	0.0680 (13)
H7A	0.3939	0.5161	0.1068	0.082*
H7B	0.3761	0.4714	0.0413	0.082*
C8	0.2907 (6)	0.3754 (4)	0.10550 (19)	0.0698 (13)
H8A	0.2160	0.3388	0.0796	0.084*
H8B	0.3904	0.3365	0.1078	0.084*
C9	0.1869 (6)	0.2907 (3)	0.1902 (2)	0.0770 (14)
H9A	0.2836	0.2490	0.1931	0.092*
H9B	0.1082	0.2543	0.1658	0.092*
C10	0.1208 (6)	0.3092 (4)	0.2507 (2)	0.0745 (14)
H10A	0.1128	0.2451	0.2725	0.089*
H10B	0.1920	0.3545	0.2730	0.089*
C11	−0.1054 (6)	0.3763 (4)	0.3006 (2)	0.0877 (16)
H11A	−0.0490	0.4326	0.3199	0.105*
H11B	−0.0995	0.3171	0.3268	0.105*
C12	−0.2778 (6)	0.4047 (4)	0.2898 (2)	0.0923 (17)
H12A	−0.3315	0.3508	0.2673	0.111*
H12B	−0.3331	0.4127	0.3280	0.111*
C13	0.3545 (4)	0.6152 (3)	0.41369 (15)	0.0440 (9)
C14	0.2763 (4)	0.6752 (2)	0.37046 (14)	0.0455 (9)
C15	0.2118 (5)	0.6326 (3)	0.31712 (16)	0.0532 (10)
C16	0.2502 (5)	0.7801 (3)	0.38195 (16)	0.0514 (10)
C17	0.0361 (7)	0.5200 (4)	0.5271 (2)	0.1024 (19)
H17A	−0.0443	0.5560	0.5507	0.123*
H17B	0.1220	0.5676	0.5171	0.123*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0458 (4)	0.0411 (4)	0.0470 (4)	0.0044 (3)	−0.0006 (3)	−0.0004 (3)
K1	0.0550 (6)	0.0498 (5)	0.0525 (5)	0.0015 (4)	−0.0030 (4)	0.0027 (4)
Cl1	0.0982 (12)	0.1102 (12)	0.1131 (11)	0.0054 (9)	0.0116 (9)	0.0209 (9)
N1	0.0550 (6)	0.0498 (5)	0.0525 (5)	0.0015 (4)	−0.0030 (4)	0.0027 (4)
N2	0.109 (3)	0.051 (2)	0.070 (2)	0.015 (2)	−0.027 (2)	0.001 (2)
O1	0.060 (2)	0.098 (3)	0.0594 (18)	−0.0012 (18)	0.0029 (15)	0.0034 (17)
O2	0.067 (2)	0.063 (2)	0.074 (2)	0.0108 (16)	−0.0034 (17)	−0.0042 (17)
O3	0.076 (2)	0.066 (2)	0.0623 (19)	−0.0012 (16)	−0.0194 (17)	0.0096 (15)
O4	0.063 (2)	0.073 (2)	0.0662 (19)	−0.0087 (16)	0.0000 (15)	0.0185 (16)
O5	0.064 (2)	0.0621 (19)	0.0545 (17)	0.0056 (15)	−0.0014 (15)	−0.0014 (15)
O6	0.068 (2)	0.071 (2)	0.0554 (18)	0.0044 (16)	−0.0046 (16)	0.0133 (15)
S1	0.0644 (7)	0.0423 (6)	0.0527 (6)	0.0048 (5)	−0.0033 (5)	−0.0047 (5)
S2	0.0583 (7)	0.0412 (6)	0.0543 (6)	0.0033 (5)	−0.0100 (5)	−0.0044 (5)
C1	0.055 (3)	0.124 (5)	0.072 (3)	0.002 (3)	0.006 (3)	−0.003 (3)

C2	0.058 (3)	0.100 (4)	0.077 (3)	0.013 (3)	−0.011 (3)	−0.022 (3)
C3	0.079 (4)	0.066 (3)	0.086 (3)	0.015 (3)	−0.033 (3)	−0.006 (3)
C4	0.089 (4)	0.070 (3)	0.079 (3)	0.000 (3)	−0.028 (3)	0.013 (3)
C5	0.111 (5)	0.066 (3)	0.067 (3)	−0.004 (3)	−0.011 (3)	0.023 (3)
C6	0.083 (4)	0.083 (4)	0.071 (3)	−0.020 (3)	−0.003 (3)	0.020 (3)
C7	0.051 (3)	0.094 (4)	0.059 (3)	−0.006 (3)	0.000 (2)	−0.006 (3)
C8	0.062 (3)	0.080 (4)	0.067 (3)	0.008 (3)	−0.003 (2)	−0.010 (3)
C9	0.077 (4)	0.061 (3)	0.093 (4)	0.021 (3)	−0.012 (3)	0.012 (3)
C10	0.080 (4)	0.073 (3)	0.071 (3)	0.008 (3)	−0.017 (3)	0.026 (3)
C11	0.099 (4)	0.111 (4)	0.054 (3)	0.004 (3)	0.003 (3)	0.026 (3)
C12	0.080 (4)	0.125 (5)	0.072 (3)	−0.004 (4)	0.023 (3)	0.025 (3)
C13	0.040 (2)	0.042 (2)	0.050 (2)	−0.0022 (17)	0.0091 (18)	−0.0034 (18)
C14	0.045 (2)	0.044 (2)	0.048 (2)	0.0009 (18)	−0.0013 (19)	−0.0036 (18)
C15	0.052 (3)	0.054 (3)	0.053 (2)	0.005 (2)	−0.006 (2)	−0.005 (2)
C16	0.056 (3)	0.054 (3)	0.044 (2)	0.002 (2)	−0.009 (2)	0.007 (2)
C17	0.070 (4)	0.113 (5)	0.125 (5)	−0.026 (3)	0.035 (4)	−0.025 (4)

Geometric parameters (Å, °)

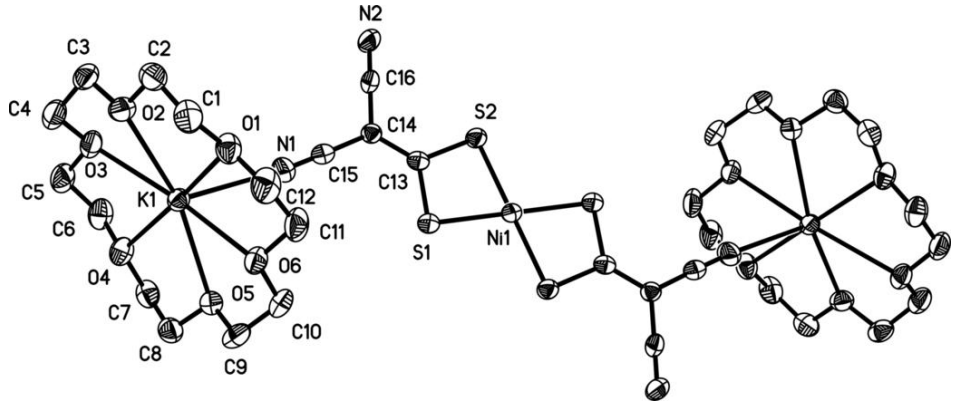
Ni1—S2^{i}	2.2101 (10)	C2—H2A	0.970
Ni1—S2	2.2101 (10)	C2—H2B	0.970
Ni1—S1	2.2170 (10)	C3—C4	1.483 (6)
Ni1—S1^{i}	2.2170 (10)	C3—H3A	0.970
K1—O6	2.727 (3)	C3—H3B	0.970
K1—O1	2.793 (3)	C4—H4A	0.970
K1—O4	2.794 (3)	C4—H4B	0.970
K1—O2	2.806 (3)	C5—C6	1.473 (6)
K1—O5	2.820 (3)	C5—H5A	0.970
K1—O3	2.828 (3)	C5—H5B	0.970
K1—N2^{ii}	2.879 (4)	C6—H6A	0.970
K1—N1	3.021 (3)	C6—H6B	0.970
Cl1—C17	1.803 (7)	C7—C8	1.476 (6)
N1—C15	1.142 (4)	C7—H7A	0.970
N2—C16	1.145 (5)	C7—H7B	0.970
N2—K1^{iii}	2.879 (4)	C8—H8A	0.970
O1—C12	1.417 (5)	C8—H8B	0.970
O1—C1	1.426 (5)	C9—C10	1.471 (6)
O2—C2	1.402 (5)	C9—H9A	0.970
O2—C3	1.406 (5)	C9—H9B	0.970
O3—C4	1.408 (5)	C10—H10A	0.970
O3—C5	1.422 (5)	C10—H10B	0.970
O4—C6	1.399 (5)	C11—C12	1.492 (6)
O4—C7	1.418 (5)	C11—H11A	0.970
O5—C8	1.401 (4)	C11—H11B	0.970
O5—C9	1.413 (5)	C12—H12A	0.970
O6—C11	1.403 (5)	C12—H12B	0.970
O6—C10	1.409 (5)	C13—C14	1.397 (3)
S1—C13	1.715 (4)	C14—C16	1.411 (4)

S2—C13	1.721 (4)	C14—C15	1.412 (3)
C1—C2	1.475 (6)	C17—C17^{iv}	1.440 (10)
C1—H1A	0.970	C17—H17A	0.970
C1—H1B	0.970	C17—H17B	0.970
S2^{i}—Ni1—S2	180	O2—C3—H3B	109.9
S2^{i}—Ni1—S1	101.71 (4)	C4—C3—H3B	109.9
S2—Ni1—S1	78.29 (4)	H3A—C3—H3B	108.3
S2^{i}—Ni1—S1^{i}	78.29 (4)	O3—C4—C3	111.4 (4)
S2—Ni1—S1^{i}	101.71 (4)	O3—C4—H4A	109.3
S1—Ni1—S1^{i}	180	C3—C4—H4A	109.3
O6—K1—O1	61.19 (9)	O3—C4—H4B	109.3
O6—K1—O4	118.91 (9)	C3—C4—H4B	109.3
O1—K1—O4	172.78 (9)	H4A—C4—H4B	108.0
O6—K1—O2	117.09 (10)	O3—C5—C6	110.9 (4)
O1—K1—O2	59.78 (9)	O3—C5—H5A	109.5
O4—K1—O2	116.91 (9)	C6—C5—H5A	109.5
O6—K1—O5	61.43 (9)	O3—C5—H5B	109.5
O1—K1—O5	122.43 (9)	C6—C5—H5B	109.5
O4—K1—O5	58.82 (8)	H5A—C5—H5B	108.1
O2—K1—O5	164.70 (9)	O4—C6—C5	108.9 (4)
O6—K1—O3	172.71 (9)	O4—C6—H6A	109.9
O1—K1—O3	117.98 (10)	C5—C6—H6A	109.9
O4—K1—O3	60.89 (9)	O4—C6—H6B	109.9
O2—K1—O3	59.83 (9)	C5—C6—H6B	109.9
O5—K1—O3	119.51 (9)	H6A—C6—H6B	108.3
O6—K1—N2^{ii}	75.36 (10)	O4—C7—C8	107.4 (4)
O1—K1—N2^{ii}	82.66 (10)	O4—C7—H7A	110.2
O4—K1—N2^{ii}	90.38 (10)	C8—C7—H7A	110.2
O2—K1—N2^{ii}	77.62 (11)	O4—C7—H7B	110.2
O5—K1—N2^{ii}	87.53 (10)	C8—C7—H7B	110.2
O3—K1—N2^{ii}	97.37 (10)	H7A—C7—H7B	108.5
O6—K1—N1	78.60 (9)	O5—C8—C7	109.6 (4)
O1—K1—N1	84.54 (9)	O5—C8—H8A	109.8
O4—K1—N1	102.62 (9)	C7—C8—H8A	109.8
O2—K1—N1	114.72 (9)	O5—C8—H8B	109.8
O5—K1—N1	80.37 (8)	C7—C8—H8B	109.8
O3—K1—N1	108.67 (9)	H8A—C8—H8B	108.2
N2^{ii}—K1—N1	153.96 (10)	O5—C9—C10	109.0 (4)
C15—N1—K1	169.6 (3)	O5—C9—H9A	109.9
C16—N2—K1^{iii}	132.7 (3)	C10—C9—H9A	109.9
C12—O1—C1	111.8 (4)	O5—C9—H9B	109.9
C12—O1—K1	114.6 (3)	C10—C9—H9B	109.9
C1—O1—K1	114.1 (2)	H9A—C9—H9B	108.3
C2—O2—C3	114.0 (4)	O6—C10—C9	108.9 (4)
C2—O2—K1	117.5 (3)	O6—C10—H10A	109.9
C3—O2—K1	117.6 (3)	C9—C10—H10A	109.9

C4—O3—C5	112.5 (3)	O6—C10—H10B	109.9
C4—O3—K1	112.8 (3)	C9—C10—H10B	109.9
C5—O3—K1	113.3 (2)	H10A—C10—H10B	108.3
C6—O4—C7	113.7 (3)	O6—C11—C12	108.5 (4)
C6—O4—K1	110.6 (3)	O6—C11—H11A	110.0
C7—O4—K1	117.7 (2)	C12—C11—H11A	110.0
C8—O5—C9	113.0 (3)	O6—C11—H11B	110.0
C8—O5—K1	114.8 (2)	C12—C11—H11B	110.0
C9—O5—K1	110.4 (2)	H11A—C11—H11B	108.4
C11—O6—C10	113.2 (3)	O1—C12—C11	109.3 (4)
C11—O6—K1	111.1 (3)	O1—C12—H12A	109.8
C10—O6—K1	114.1 (2)	C11—C12—H12A	109.8
C13—S1—Ni1	86.39 (12)	O1—C12—H12B	109.8
C13—S2—Ni1	86.45 (12)	C11—C12—H12B	109.8
O1—C1—C2	110.4 (4)	H12A—C12—H12B	108.3
O1—C1—H1A	109.6	C14—C13—S1	126.2 (3)
C2—C1—H1A	109.6	C14—C13—S2	124.9 (3)
O1—C1—H1B	109.6	S1—C13—S2	108.9 (2)
C2—C1—H1B	109.6	C13—C14—C16	119.4 (3)
H1A—C1—H1B	108.1	C13—C14—C15	121.9 (3)
O2—C2—C1	109.6 (4)	C16—C14—C15	118.5 (3)
O2—C2—H2A	109.7	N1—C15—C14	178.0 (4)
C1—C2—H2A	109.7	N2—C16—C14	179.9 (5)
O2—C2—H2B	109.7	C17^{iv}—C17—Cl1	108.1 (6)
C1—C2—H2B	109.7	C17^{iv}—C17—H17A	110.1
H2A—C2—H2B	108.2	Cl1—C17—H17A	110.1
O2—C3—C4	109.1 (4)	C17^{iv}—C17—H17B	110.1
O2—C3—H3A	109.9	Cl1—C17—H17B	110.1
C4—C3—H3A	109.9	H17A—C17—H17B	108.4

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

Fig. 1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C1
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O3
C15
C13
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C6
C11
S1
Ni1
O4
O6
O5
C7
C10
C8
C9

Fig. 2

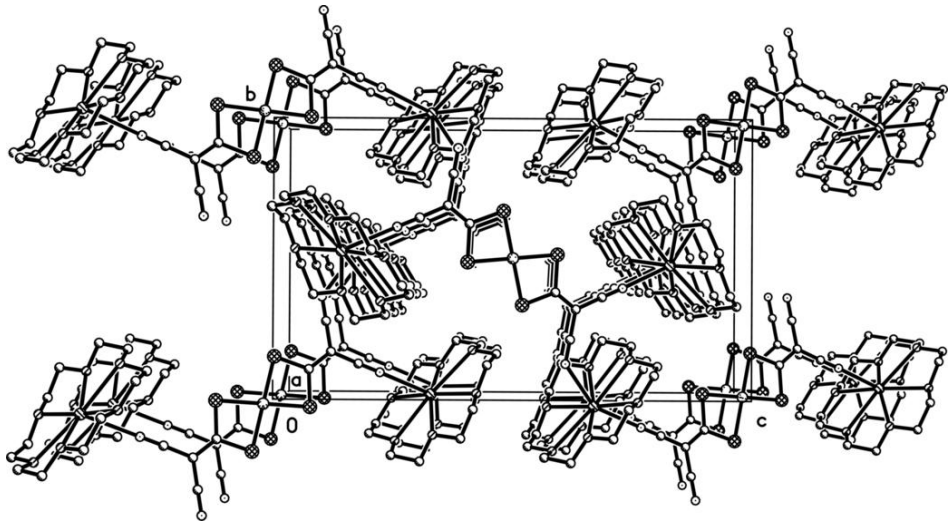

Fig. 3