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Bis(18-crown-6)-1κ^6O,3κ^6O-bis(μ-1,1-dicyanoethylene-2,2-dithiolato)-1:2κ^3N:S,S';2:3κ^3S,S':N-dipotassium(I)-copper(II) 1,2-dichloroethane solvate

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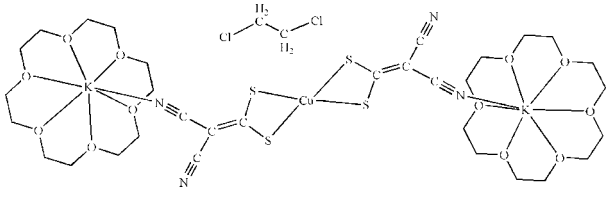
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.013 Å; R factor = 0.056; wR factor = 0.170; data-to-parameter ratio = 16.0.

In the title complex, $[CuK_2(C_4N_2S_2)_2(C_{12}H_{24}O_6)_2]\cdot C_2H_4Cl_2$, the Cu^{II} atom lies on an inversion centre and the 1,2-dichloroethane solvate lies on another inversion centre. The asymmetric unit therefore comprises one $[K(18\text{-crown-6})]^+$ complex cation, one-half of the $[Cu(i\text{-mnt})_2]^{2-}$ anion (i-mnt is 1,1-dicyanoethylene-2,2-dithiolate) and one-half of the dichloroethane solvent molecule. Each K^I ion binds to the six ether O atoms and N atoms from two i-mnt^{2-} ligands. The Cu atoms adopt a distorted square-planar coordination geometry. K—N bonds from each of the four cyano groups link the cations and anions into planar sheets along the diagonal of the *ac* plane and these sheets pack in layers in the *bc* plane.

Related literature

For applications of coordination polymers, see: Chen & Suslick (1993); for the structures and applications of crown ether transition metal bis(dithiolate) salts, see: Long *et al.* (1998) and Nakamura *et al.* (1998).



Experimental

Crystal data

$[CuK_2(C_4N_2S_2)_2(C_{12}H_{24}O_6)_2]\cdot C_2H_4Cl_2$
M_r = 1049.68
Monoclinic, $P2_1/c$
a = 8.259 (3) Å
b = 13.084 (4) Å
c = 22.228 (7) Å
β = 90.413 (6)°
V = 2401.8 (13) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.97 mm^{-1}
T = 293 (2) K
0.22 × 0.15 × 0.07 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.815, T_{max} = 0.935
12535 measured reflections
4281 independent reflections
1698 reflections with $I > 2\sigma(I)$
R_{int} = 0.084

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.171
S = 1.00
4281 reflections
268 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); 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: SJ2302).

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supplementary materials

Acta Cryst. (2007). E**63**, m1522 [**doi:10.1107/S1600536807020028**]

Bis(18-crown-6)-1κ^6O,3κ^6O-bis(μ-1,1-dicyanoethylene-2,2-dithiolato)-1:2κ^3N:*S*,*S*';2:3κ^3S,*S*':*N*-dipotassium(I)copper(II) 1,2-dichloroethane solvate

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

Comment

In recent years, metal coordination complexes with polymeric structures have attracted interest owing to their important applications as materials with unusual properties (Chen *et al.*, 1993). The complexes formed by crown ether cations and transition metal bis(dithiolate) salts, including 1,1-dicyanoethylene-2,2dithiolate (i-mnt^{2-}) (Long *et al.*, 1998) have attracted widespread interest due to their novel structures and unusual electrical, magnetic and optical properties (Nakamura *et al.*, 1998). We report here one such novel complex [K(18Crown-6)]$_2$[Cu(i-mnt)$_2$], Fig. 1.

In the title complex, the Cu^{II} atom lies on an inversion centre while the 1,2-dichloroethane solvate lies about an inversion centre. The asymmetric unit therefore comprises one [K(18Crown-6)]$^+$ cation, one half of the [Cu(i-mnt)$_2$]$^{2-}$ anion (i-mnt = 1,1-dicyanoethylene-2,2dithiolate) and one half of the dichloroethane solvate. In the cation [K(18Crown-6)]$^+$, the potassium ion lies within the crown ether cage with K—O bond lengths in the range 2.722 (5) to 2.826 (5) Å. The K$^+$ ion lies 0.2210Å out of meanplane through the six ether O atoms. Each K$^+$ ion also binds in a *trans* configuration to two N atoms from adjacent i-mnt ligands with K—N distances 2.828 (7) and 2.963 (7) Å. The Cu atoms adopt a distorted square planar coordination geometry with Cu—S distances 2.302 (2) and 2.3324 (19) Å. In the crystal structure, K—N bonds from each of the four cyano- groups link the cations and anions into planar sheets along the diagonal of the *ac* plane, Fig 2, and these sheets pack in layers in the *bc* plane, Fig. 3.

Experimental

To a solution of 18-crown-6 (2.0 mmol) in 1,2-dichloroethane (10.0 ml) was added 5 ml 1,2-dichloroethane mixture of $CuCl_2$ (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 (*v*/*v*) diethyl ether/ 1,2-dichloroethane and colorless single crystals were obtained by slowly evaporating this solution. Elemental analysis found: H 4.99, C 38.90, N 5.34%; calculated for $C_{34}H_{52}Cl_2K_2N_4O_{12}S_4Cu$: H 4.87, C 38.95, N 5.22%.

Refinement

All H-atoms were positioned geometrically and refined using a riding model with d(C—H) = 0.97 Å, U_{iso} = 1.2U_{eq} (C) for the CH_2 atoms.

Figures

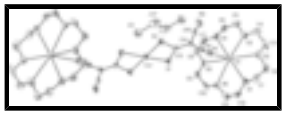


Fig. 1. The structure of the title complex, showing 30% probability displacement ellipsoids and the atom-numbering scheme. Labelled atoms are related to unlabelled atoms by the symmetry operations ($1-x$, $-y$, $1-z$) for the complex and ($-x$, $1-y$, $1-z$) for the solvate molecule. H atoms have been omitted for clarity.

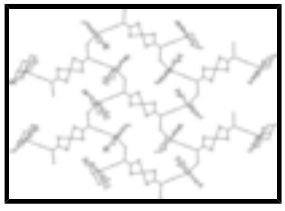


Fig. 2. The two-dimensional chain network of the title complex.

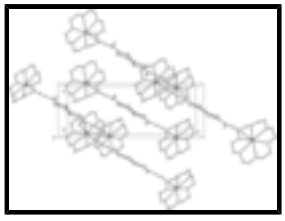


Fig. 3. Crystal packing of the title complex.

Bis(18-crown-6)–1κ^6*O*,3κ^6*O*-bis(μ-1,1-dicyanoethylene-2,2-dithiolato)- 1:2κ^3*N*:*S*,*S*';2:3κ^3*S*,*S*':*N*-dipotassium(I)copper(II) 1,2-dichloroethane solvate

Crystal data

$[CuK_2(C_4N_2S_2)_2(C_{12}H_{24}O_6)_2]\cdot C_2H_4Cl_2$	F_{000} = 1090
M_r = 1049.68	D_x = 1.451 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 1005 reflections
a = 8.259 (3) Å	θ = 2.4–18º
b = 13.084 (4) Å	μ = 0.97 mm^{-1}
c = 22.228 (7) Å	T = 293 (2) K
β = 90.413 (6)º	Block, colourless
V = 2401.8 (13) Å^3	0.22 × 0.15 × 0.07 mm
Z = 2	

Data collection

Siemens SMART CCD area-detector diffractometer	4281 independent reflections
Radiation source: fine-focus sealed tube	1698 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.084
T = 293(2) K	θ_{max} = 25.1º
φ and ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	h = −9→9
T_{min} = 0.815, T_{max} = 0.935	k = −11→15

12535 measured reflections	$l = -23 \rightarrow 26$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.056$	H-atom parameters constrained
$wR(F^2) = 0.171$	$w = 1/[\sigma^2(F_o^2) + (0.051P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} < 0.001$
4281 reflections	$\Delta\rho_{max} = 0.51$ e Å^{-3}
268 parameters	$\Delta\rho_{min} = -0.44$ 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}
Cu1	0.5000	0.5000	0.5000	0.0482 (4)
K1	−0.0443 (2)	0.47985 (13)	0.82898 (7)	0.0514 (5)
Cl1	0.1390 (3)	0.5783 (2)	0.43296 (12)	0.1075 (10)
N1	0.1485 (8)	0.3983 (5)	0.7278 (3)	0.070 (2)
N2	0.2218 (9)	0.1339 (6)	0.6114 (3)	0.077 (2)
O1	0.1706 (7)	0.4726 (5)	0.9259 (2)	0.0674 (16)
O2	−0.0850 (7)	0.3246 (4)	0.9160 (2)	0.0665 (16)
O3	−0.3476 (7)	0.3877 (4)	0.8427 (3)	0.0720 (18)
O4	−0.2879 (6)	0.5039 (5)	0.7438 (2)	0.0705 (16)
O5	−0.0337 (7)	0.6458 (4)	0.7553 (2)	0.0641 (16)
O6	0.2236 (6)	0.6121 (4)	0.8357 (2)	0.0595 (15)
S1	0.3801 (2)	0.51358 (15)	0.59435 (8)	0.0539 (6)
S2	0.4227 (2)	0.33487 (15)	0.52112 (9)	0.0527 (6)
C1	0.1820 (11)	0.3747 (8)	0.9473 (4)	0.080 (3)
H1A	0.2572	0.3726	0.9810	0.096*
H1B	0.2230	0.3301	0.9160	0.096*
C2	0.0208 (12)	0.3385 (7)	0.9668 (4)	0.083 (3)

H2A	0.0324	0.2743	0.9881	0.100*
H2B	−0.0261	0.3880	0.9941	0.100*
C3	−0.2536 (12)	0.3101 (7)	0.9293 (4)	0.097 (4)
H3A	−0.2917	0.3673	0.9530	0.116*
H3B	−0.2660	0.2486	0.9531	0.116*
C4	−0.3541 (11)	0.3014 (9)	0.8742 (4)	0.088 (3)
H4A	−0.3153	0.2451	0.8499	0.106*
H4B	−0.4654	0.2872	0.8851	0.106*
C5	−0.4536 (11)	0.3868 (8)	0.7928 (4)	0.083 (3)
H5A	−0.5629	0.3719	0.8058	0.100*
H5B	−0.4209	0.3344	0.7645	0.100*
C6	−0.4481 (10)	0.4870 (8)	0.7642 (4)	0.077 (3)
H6A	−0.5234	0.4894	0.7305	0.092*
H6B	−0.4783	0.5396	0.7927	0.092*
C7	−0.2805 (11)	0.5978 (9)	0.7127 (4)	0.090 (3)
H7A	−0.3321	0.6508	0.7363	0.108*
H7B	−0.3382	0.5921	0.6746	0.108*
C8	−0.1091 (12)	0.6258 (7)	0.7016 (4)	0.086 (3)
H8A	−0.0545	0.5700	0.6814	0.103*
H8B	−0.1044	0.6856	0.6759	0.103*
C9	0.1212 (11)	0.6881 (7)	0.7491 (4)	0.070 (3)
H9A	0.1141	0.7517	0.7268	0.084*
H9B	0.1895	0.6414	0.7268	0.084*
C10	0.1904 (11)	0.7066 (7)	0.8072 (4)	0.076 (3)
H10A	0.2896	0.7456	0.8032	0.092*
H10B	0.1156	0.7460	0.8313	0.092*
C11	0.2911 (10)	0.6221 (7)	0.8912 (4)	0.070 (3)
H11A	0.2189	0.6609	0.9167	0.085*
H11B	0.3921	0.6596	0.8881	0.085*
C12	0.3222 (10)	0.5218 (8)	0.9184 (3)	0.072 (3)
H12A	0.3913	0.4813	0.8925	0.087*
H12B	0.3761	0.5299	0.9570	0.087*
C13	0.3473 (8)	0.3831 (5)	0.5889 (3)	0.0432 (19)
C14	0.2677 (8)	0.3243 (6)	0.6315 (3)	0.0429 (19)
C15	0.2029 (9)	0.3687 (6)	0.6860 (4)	0.048 (2)
C16	0.2446 (9)	0.2183 (7)	0.6194 (3)	0.049 (2)
C17	0.0317 (12)	0.4761 (9)	0.4737 (4)	0.125 (4)
H17A	−0.0552	0.4481	0.4491	0.150*
H17B	0.1055	0.4213	0.4845	0.150*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0521 (9)	0.0443 (9)	0.0482 (8)	−0.0080 (7)	0.0057 (6)	0.0008 (7)
K1	0.0541 (11)	0.0500 (12)	0.0502 (10)	0.0015 (9)	0.0052 (8)	0.0039 (9)
Cl1	0.092 (2)	0.118 (3)	0.113 (2)	−0.0143 (18)	−0.0027 (17)	0.0193 (19)
N1	0.080 (6)	0.078 (6)	0.052 (5)	−0.011 (4)	0.022 (4)	−0.010 (4)
N2	0.111 (6)	0.049 (5)	0.072 (5)	−0.016 (5)	0.034 (4)	0.000 (4)

O1	0.072 (4)	0.064 (4)	0.067 (4)	0.015 (3)	0.001 (3)	0.021 (3)
O2	0.077 (4)	0.063 (4)	0.059 (4)	0.007 (3)	0.012 (3)	0.009 (3)
O3	0.080 (5)	0.048 (4)	0.088 (5)	−0.008 (4)	0.013 (4)	0.012 (4)
O4	0.055 (4)	0.096 (5)	0.060 (4)	0.003 (4)	0.004 (3)	0.010 (4)
O5	0.065 (4)	0.075 (4)	0.052 (4)	−0.005 (3)	0.002 (3)	0.010 (3)
O6	0.063 (4)	0.071 (4)	0.044 (3)	−0.004 (3)	0.001 (3)	0.000 (3)
S1	0.0668 (14)	0.0437 (13)	0.0513 (12)	−0.0061 (11)	0.0078 (10)	−0.0024 (11)
S2	0.0616 (14)	0.0426 (13)	0.0542 (12)	−0.0051 (11)	0.0134 (10)	−0.0045 (10)
C1	0.076 (7)	0.092 (8)	0.072 (6)	0.026 (6)	0.003 (5)	0.004 (6)
C2	0.122 (9)	0.054 (6)	0.074 (7)	0.016 (6)	0.015 (7)	0.028 (5)
C3	0.098 (8)	0.057 (7)	0.136 (10)	0.015 (6)	0.081 (8)	0.035 (7)
C4	0.054 (6)	0.125 (11)	0.087 (8)	−0.008 (7)	0.011 (6)	−0.045 (8)
C5	0.061 (7)	0.125 (10)	0.063 (6)	−0.012 (6)	0.000 (5)	−0.021 (6)
C6	0.054 (6)	0.116 (9)	0.061 (6)	0.010 (6)	−0.003 (4)	0.012 (6)
C7	0.069 (8)	0.147 (11)	0.053 (6)	−0.004 (7)	−0.015 (5)	0.013 (6)
C8	0.105 (9)	0.095 (8)	0.058 (6)	−0.001 (7)	0.006 (6)	0.028 (6)
C9	0.072 (7)	0.076 (7)	0.063 (6)	0.001 (6)	0.002 (5)	0.019 (5)
C10	0.074 (7)	0.058 (7)	0.097 (8)	−0.019 (5)	0.016 (6)	0.016 (6)
C11	0.058 (6)	0.053 (6)	0.101 (8)	−0.001 (5)	0.025 (6)	−0.004 (6)
C12	0.043 (6)	0.116 (9)	0.058 (5)	0.005 (6)	−0.002 (4)	−0.019 (6)
C13	0.036 (4)	0.044 (5)	0.050 (5)	0.005 (4)	−0.001 (4)	−0.007 (4)
C14	0.040 (5)	0.038 (5)	0.051 (5)	−0.006 (4)	0.005 (4)	0.010 (4)
C15	0.049 (5)	0.047 (5)	0.046 (5)	−0.007 (4)	−0.002 (4)	0.009 (4)
C16	0.055 (5)	0.055 (6)	0.037 (5)	−0.008 (5)	0.013 (4)	0.009 (5)
C17	0.074 (8)	0.150 (13)	0.151 (12)	0.040 (7)	−0.040 (8)	−0.038 (9)

Geometric parameters (Å, °)

Cu1—S2	2.302 (2)	C1—H1B	0.9700
Cu1—S2^{i}	2.302 (2)	C2—H2A	0.9700
Cu1—S1^{i}	2.3324 (19)	C2—H2B	0.9700
Cu1—S1	2.3324 (19)	C3—C4	1.478 (11)
K1—O5	2.722 (5)	C3—H3A	0.9700
K1—O4	2.771 (6)	C3—H3B	0.9700
K1—O1	2.783 (5)	C4—H4A	0.9700
K1—O3	2.798 (6)	C4—H4B	0.9700
K1—O6	2.812 (6)	C5—C6	1.459 (11)
K1—O2	2.826 (5)	C5—H5A	0.9700
K1—N2^{ii}	2.828 (7)	C5—H5B	0.9700
K1—N1	2.963 (7)	C6—H6A	0.9700
K1—C8	3.454 (8)	C6—H6B	0.9700
K1—C1	3.497 (9)	C7—C8	1.485 (11)
K1—C9	3.533 (9)	C7—H7A	0.9700
Cl1—C17	1.846 (13)	C7—H7B	0.9700
N1—C15	1.107 (8)	C8—H8A	0.9700
N2—C16	1.134 (9)	C8—H8B	0.9700
N2—K1^{iii}	2.828 (7)	C9—C10	1.429 (10)
O1—C1	1.370 (9)	C9—H9A	0.9700

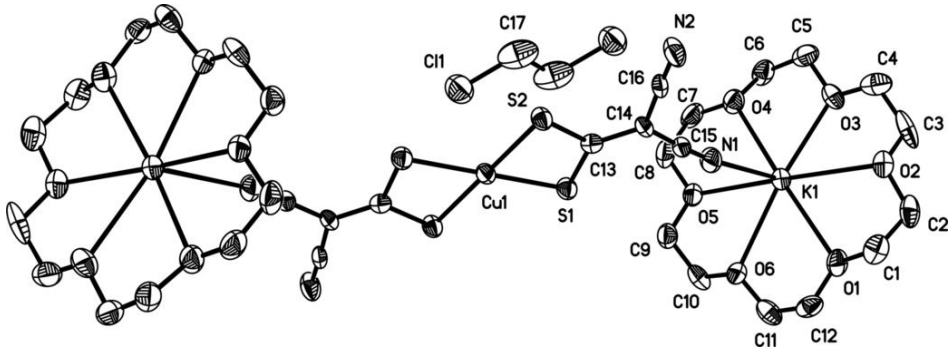
O1—C12	1.419 (9)	C9—H9B	0.9700
O2—C2	1.433 (9)	C10—H10A	0.9700
O2—C3	1.438 (9)	C10—H10B	0.9700
O3—C4	1.330 (11)	C11—C12	1.468 (10)
O3—C5	1.407 (9)	C11—H11A	0.9700
O4—C7	1.411 (10)	C11—H11B	0.9700
O4—C6	1.419 (9)	C12—H12A	0.9700
O5—C8	1.368 (9)	C12—H12B	0.9700
O5—C9	1.401 (9)	C13—C14	1.390 (9)
O6—C11	1.357 (9)	C14—C16	1.425 (10)
O6—C10	1.415 (9)	C14—C15	1.448 (10)
S1—C13	1.733 (7)	C17—C17^{iv}	1.430 (17)
S2—C13	1.751 (7)	C17—H17A	0.9700
C1—C2	1.481 (11)	C17—H17B	0.9700
C1—H1A	0.9700		
S2—Cu1—S2^{i}	180.000 (1)	C2—C1—H1B	109.7
S2—Cu1—S1^{i}	103.42 (7)	K1—C1—H1B	83.4
S2^{i}—Cu1—S1^{i}	76.58 (7)	H1A—C1—H1B	108.2
S2—Cu1—S1	76.58 (7)	O2—C2—C1	110.8 (7)
S2^{i}—Cu1—S1	103.42 (7)	O2—C2—H2A	109.5
S1^{i}—Cu1—S1	180.000 (1)	C1—C2—H2A	109.5
O5—K1—O4	61.60 (18)	O2—C2—H2B	109.5
O5—K1—O1	118.01 (19)	C1—C2—H2B	109.5
O4—K1—O1	171.42 (17)	H2A—C2—H2B	108.1
O5—K1—O3	116.23 (19)	O2—C3—C4	112.3 (7)
O4—K1—O3	58.50 (18)	O2—C3—H3A	109.2
O1—K1—O3	117.87 (19)	C4—C3—H3A	109.2
O5—K1—O6	60.79 (17)	O2—C3—H3B	109.2
O4—K1—O6	122.23 (18)	C4—C3—H3B	109.2
O1—K1—O6	58.85 (17)	H3A—C3—H3B	107.9
O3—K1—O6	164.57 (17)	O3—C4—C3	110.3 (9)
O5—K1—O2	171.73 (16)	O3—C4—H4A	109.6
O4—K1—O2	117.40 (19)	C3—C4—H4A	109.6
O1—K1—O2	61.59 (18)	O3—C4—H4B	109.6
O3—K1—O2	60.33 (18)	C3—C4—H4B	109.6
O6—K1—O2	120.23 (18)	H4A—C4—H4B	108.1
O5—K1—N2^{ii}	74.48 (18)	O3—C5—C6	108.4 (8)
O4—K1—N2^{ii}	82.2 (2)	O3—C5—H5A	110.0
O1—K1—N2^{ii}	89.5 (2)	C6—C5—H5A	110.0
O3—K1—N2^{ii}	77.8 (2)	O3—C5—H5B	110.0
O6—K1—N2^{ii}	87.0 (2)	C6—C5—H5B	110.0
O2—K1—N2^{ii}	97.27 (18)	H5A—C5—H5B	108.4
O5—K1—N1	79.11 (18)	O4—C6—C5	108.1 (7)
O4—K1—N1	85.06 (18)	O4—C6—H6A	110.1
O1—K1—N1	103.39 (18)	C5—C6—H6A	110.1
O3—K1—N1	114.45 (19)	O4—C6—H6B	110.1

O6—K1—N1	80.48 (17)	C5—C6—H6B	110.1
O2—K1—N1	109.13 (18)	H6A—C6—H6B	108.4
N2^{ii}—K1—N1	153.6 (2)	O4—C7—C8	109.9 (8)
O5—K1—C8	21.73 (18)	O4—C7—H7A	109.7
O4—K1—C8	43.1 (2)	C8—C7—H7A	109.7
O1—K1—C8	138.4 (2)	O4—C7—H7B	109.7
O3—K1—C8	101.2 (2)	C8—C7—H7B	109.7
O6—K1—C8	79.6 (2)	H7A—C7—H7B	108.2
O2—K1—C8	160.0 (2)	O5—C8—C7	109.3 (7)
N2^{ii}—K1—C8	85.0 (2)	O5—C8—K1	47.4 (4)
N1—K1—C8	70.0 (2)	C7—C8—K1	82.5 (5)
O5—K1—C1	138.3 (2)	O5—C8—H8A	109.8
O4—K1—C1	160.1 (2)	C7—C8—H8A	109.8
O1—K1—C1	21.59 (18)	K1—C8—H8A	84.0
O3—K1—C1	102.9 (2)	O5—C8—H8B	109.8
O6—K1—C1	77.7 (2)	C7—C8—H8B	109.8
O2—K1—C1	43.0 (2)	K1—C8—H8B	157.3
N2^{ii}—K1—C1	101.8 (2)	H8A—C8—H8B	108.3
N1—K1—C1	98.1 (2)	O5—C9—C10	109.7 (7)
C8—K1—C1	155.9 (2)	C10—C9—K1	80.2 (5)
O5—K1—C9	21.24 (16)	O5—C9—H9A	109.7
O4—K1—C9	81.4 (2)	C10—C9—H9A	109.7
O1—K1—C9	99.7 (2)	K1—C9—H9A	153.7
O3—K1—C9	137.5 (2)	O5—C9—H9B	109.7
O6—K1—C9	40.96 (18)	C10—C9—H9B	109.7
O2—K1—C9	161.2 (2)	K1—C9—H9B	90.0
N2^{ii}—K1—C9	83.7 (2)	H9A—C9—H9B	108.2
N1—K1—C9	71.6 (2)	O6—C10—C9	109.4 (8)
C8—K1—C9	38.7 (2)	O6—C10—H10A	109.8
C1—K1—C9	118.3 (2)	C9—C10—H10A	109.8
C15—N1—K1	171.1 (7)	O6—C10—H10B	109.8
C16—N2—K1^{iii}	134.9 (6)	C9—C10—H10B	109.8
C1—O1—C12	114.0 (7)	H10A—C10—H10B	108.3
C1—O1—K1	110.0 (5)	O6—C11—C12	111.0 (7)
C12—O1—K1	116.9 (4)	O6—C11—H11A	109.4
C2—O2—C3	116.1 (7)	C12—C11—H11A	109.4
C2—O2—K1	111.9 (5)	O6—C11—H11B	109.4
C3—O2—K1	110.8 (5)	C12—C11—H11B	109.4
C4—O3—C5	112.4 (8)	H11A—C11—H11B	108.0
C4—O3—K1	117.6 (6)	O1—C12—C11	107.6 (7)
C5—O3—K1	118.1 (5)	O1—C12—H12A	110.2
C7—O4—C6	109.6 (7)	C11—C12—H12A	110.2
C7—O4—K1	113.6 (5)	O1—C12—H12B	110.2
C6—O4—K1	116.0 (4)	C11—C12—H12B	110.2
C8—O5—C9	113.5 (7)	H12A—C12—H12B	108.5
C8—O5—K1	110.8 (5)	C14—C13—S1	124.9 (5)
C9—O5—K1	114.1 (5)	C14—C13—S2	124.0 (6)
C11—O6—C10	113.6 (7)	S1—C13—S2	111.1 (4)

C11—O6—K1	115.2 (5)	C13—C14—C16	118.2 (7)
C10—O6—K1	111.3 (5)	C13—C14—C15	121.8 (7)
C13—S1—Cu1	85.9 (2)	C16—C14—C15	119.9 (6)
C13—S2—Cu1	86.4 (3)	N1—C15—C14	176.4 (9)
O1—C1—C2	109.9 (7)	N2—C16—C14	177.4 (8)
O1—C1—K1	48.4 (4)	$C17^{iv}$—C17—Cl1	105.3 (12)
C2—C1—K1	82.5 (5)	$C17^{iv}$—C17—H17A	110.7
O1—C1—H1A	109.7	Cl1—C17—H17A	110.7
C2—C1—H1A	109.7	$C17^{iv}$—C17—H17B	110.7
K1—C1—H1A	158.1	Cl1—C17—H17B	110.7
O1—C1—H1B	109.7	H17A—C17—H17B	108.8

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*, *y*+1/2, −*z*+3/2; (iii) −*x*, *y*−1/2, −*z*+3/2; (iv) −*x*, −*y*+1, −*z*+1.

Fig. 1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C13
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O1
C1
C10
C11
C12

Fig. 2

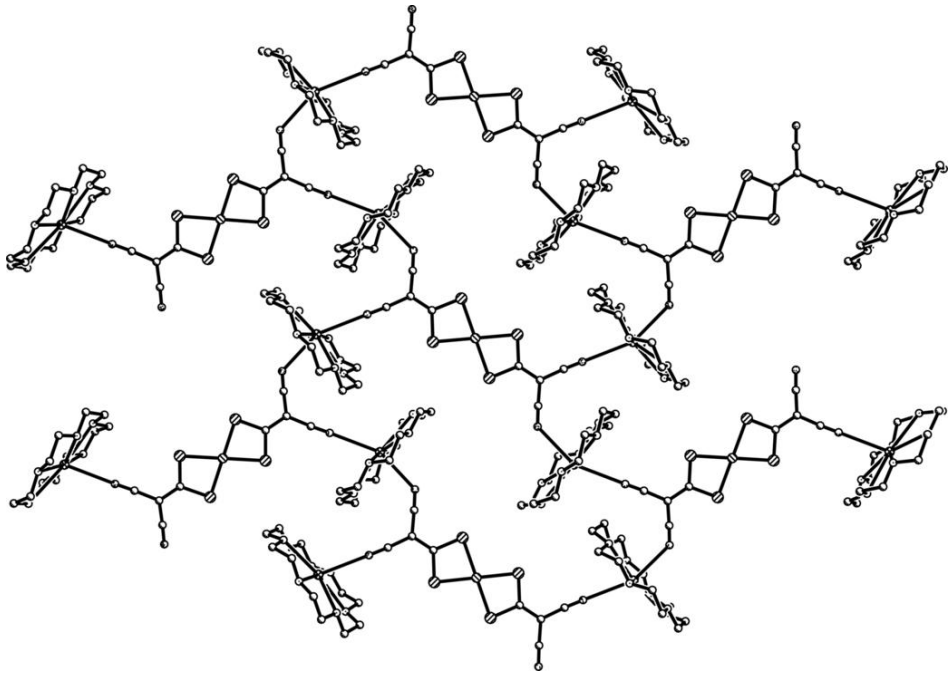

Fig. 3