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catena-Poly[[(18-crown-6)potassium(I)]-μ-chlorido-silver(I)-μ-chlorido]

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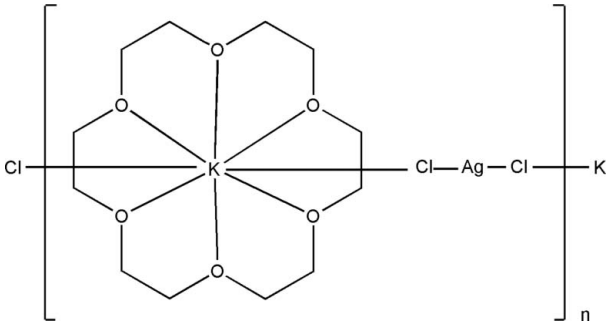
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.027; wR factor = 0.079; data-to-parameter ratio = 16.5.

The title complex, $[AgKCl_2(C_{12}H_{24}O_6)]_n$, has been synthesized by reaction of 18-crown-6 with KCl and $AgNO_3$. $[K(18\text{-crown-6})]^+$ cations and $[AgCl_2]^-$ anions form one-dimensional chains through K$\cdots$Cl interactions of length 3.2568 (14) Å. Both the K^+ and the Ag^I ions lie on centres of inversion.

Related literature

For other examples of structures incorporating $[AgCl_2]^-$ anions, see: Exarchos *et al.* (1998); Gerisch *et al.* (1997). For polymeric structures incorporating crown ethers, see: Desai *et al.* (2001); Bastos *et al.* (2000).



Experimental

Crystal data

$[AgKCl_2(C_{12}H_{24}O_6)]$
M_r = 482.18
Monoclinic, $P2_1/n$
a = 8.691 (4) Å
b = 8.244 (4) Å
c = 13.833 (6) Å
β = 102.764 (6)°
V = 966.6 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.56 mm^{-1}
T = 298 (2) K
0.56 × 0.34 × 0.30 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.457, T_{max} = 0.627
4877 measured reflections
1699 independent reflections
1308 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.079
S = 1.03
1699 reflections
103 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); 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, 1997); 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: BI2208).

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supplementary materials

Acta Cryst. (2007). E**63**, m2219 [**doi:10.1107/S1600536807035726**]

catena-Poly[[(18-crown-6)potassium(I)]-μ-chlorido-silver(I)-μ-chlorido]

X.-M. Song, X.-Q. Huang, J.-M. Dou and D.-C. Li

Comment

Much interest has been focused on crown ethers and their metal cations because they can act as modules to form novel polymeric structures (Desai *et al.*, 2001; Bastos *et al.*, 2000). The title complex consists of $[K(18\text{-crown-6})]^+$ cations linked by $[AgCl_2]^-$ anions (Figure 1).

The Ag^I atom lies on a centre of inversion and is coordinated in a linear manner by by two Cl atoms with an Ag—Cl bond length of 2.3114 (10) Å. In the $[K(18\text{-crown-6})]^+$ cation, K^+ lies on a centre of inversion and is coordinated by six O atoms, with K^+ lying approximately in the plane of the crown ether. The K—O bond lengths vary from 2.783 (2) to 2.830 (2) Å. The cations and anions are linked *via* K—Cl interactions of length 3.2568 (14) Å, forming one-dimensional chains along the *b* axis (Figure 2).

Experimental

KCl (0.2238 g, 3.0 mmol) and $AgNO_3$ (0.2548 g,1.5 mmol) in 15 ml e thanol were refluxed for 4 h, then 18-crown-6 (0.421 g, 1.5 mmol) was added slowly and the mixture was refluxed for a further 4 h. After cooling to room temperature, the mixture was filtered and the resulting solid was recrystallized from ether. Elemental analysis: calculated C 29.89, H 4.98%; found: C 30.02, H 4.99.

Refinement

H atoms were positioned geometrically and refined using a riding model with C—H = 0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

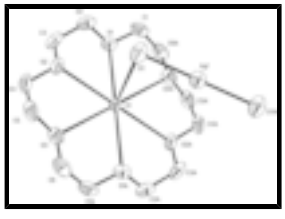

Fig. 1. Molecular structure of the title compound showing displacement ellipsoids at the 30% probability level. H atoms are omitted. Symmetry code (A): $1-x, 1-y, 1-z$.

Fig. 2. One-dimensional chain running along the *b*-axis.

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Crystal data

$[AgKCl_2(C_{12}H_{24}O_6)]$	$F_{000} = 488$
$M_r = 482.18$	$D_x = 1.657$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 2464 reflections
$a = 8.691$ (4) Å	$\theta = 2.9$–26.1º
$b = 8.244$ (4) Å	$\mu = 1.56$ mm^{-1}
$c = 13.833$ (6) Å	$T = 298$ (2) K
$\beta = 102.764$ (6)º	Block, colourless
$V = 966.6$ (8) Å^3	0.56 × 0.34 × 0.30 mm
$Z = 2$	

Data collection

Bruker SMART CCD diffractometer	1699 independent reflections
Radiation source: fine-focus sealed tube	1308 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.020$
$T = 298$(2) K	$\theta_{max} = 25.0$º
φ and ω scans	$\theta_{min} = 2.5$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -6 \rightarrow 10$
$T_{min} = 0.457$, $T_{max} = 0.627$	$k = -9 \rightarrow 9$
4877 measured reflections	$l = -15 \rightarrow 16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.027$	H-atom parameters constrained
$wR(F^2) = 0.079$	$w = 1/[\sigma^2(F_o^2) + (0.0449P)^2 + 0.1659P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} < 0.001$
1699 reflections	$\Delta\rho_{max} = 0.20$ e Å^{-3}
103 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}
Cl1	0.68538 (10)	0.17256 (10)	0.45904 (7)	0.0811 (3)
Ag1	0.5000	0.0000	0.5000	0.06429 (16)
K1	0.5000	0.5000	0.5000	0.0469 (2)
O1	0.5045 (3)	0.5512 (2)	0.29837 (13)	0.0602 (5)
O2	0.7752 (2)	0.6133 (2)	0.45167 (15)	0.0629 (5)
O3	0.7445 (2)	0.6290 (2)	0.64818 (13)	0.0624 (5)
C1	0.4100 (4)	0.4327 (4)	0.2368 (2)	0.0764 (10)
H1A	0.4570	0.3261	0.2510	0.092*
H1B	0.4053	0.4573	0.1677	0.092*
C2	0.6609 (4)	0.5529 (4)	0.2855 (2)	0.0704 (9)
H2A	0.6617	0.5810	0.2176	0.084*
H2B	0.7074	0.4461	0.2992	0.084*
C3	0.7541 (4)	0.6736 (4)	0.3540 (2)	0.0722 (9)
H3A	0.8557	0.6905	0.3375	0.087*
H3B	0.6988	0.7765	0.3483	0.087*
C4	0.8766 (4)	0.7074 (4)	0.5233 (3)	0.0775 (10)
H4A	0.8337	0.8158	0.5251	0.093*
H4B	0.9792	0.7162	0.5070	0.093*
C5	0.8922 (3)	0.6288 (4)	0.6205 (3)	0.0782 (10)
H5A	0.9286	0.5181	0.6172	0.094*
H5B	0.9695	0.6865	0.6698	0.094*
C6	0.7508 (4)	0.5672 (5)	0.7444 (2)	0.0775 (10)
H6A	0.8198	0.6339	0.7932	0.093*
H6B	0.7925	0.4576	0.7495	0.093*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0670 (5)	0.0692 (5)	0.1129 (7)	0.0011 (4)	0.0325 (5)	0.0147 (4)
Ag1	0.0596 (2)	0.0636 (2)	0.0702 (2)	−0.00286 (15)	0.01553 (17)	0.00199 (15)
K1	0.0389 (4)	0.0580 (5)	0.0438 (4)	−0.0085 (3)	0.0093 (3)	−0.0009 (3)
O1	0.0699 (13)	0.0619 (11)	0.0505 (11)	0.0093 (10)	0.0171 (10)	0.0017 (9)

O2	0.0523 (11)	0.0603 (12)	0.0785 (13)	−0.0153 (10)	0.0193 (10)	0.0032 (10)
O3	0.0484 (11)	0.0703 (12)	0.0614 (12)	0.0053 (9)	−0.0029 (9)	−0.0083 (9)
C1	0.110 (3)	0.0723 (19)	0.0434 (16)	0.006 (2)	0.0098 (18)	−0.0033 (15)
C2	0.089 (2)	0.0700 (18)	0.0629 (19)	0.0200 (19)	0.0393 (18)	0.0167 (16)
C3	0.0593 (18)	0.0677 (19)	0.102 (3)	0.0081 (16)	0.0450 (19)	0.0265 (18)
C4	0.0480 (17)	0.068 (2)	0.121 (3)	−0.0186 (16)	0.0290 (19)	−0.019 (2)
C5	0.0355 (15)	0.086 (2)	0.104 (3)	−0.0010 (15)	−0.0050 (16)	−0.032 (2)
C6	0.083 (3)	0.073 (2)	0.063 (2)	0.0062 (18)	−0.0147 (18)	−0.0048 (15)

Geometric parameters (Å, °)

Cl1—Ag1	2.3117 (11)	C1—C6^{ii}	1.477 (4)
Cl1—K1	3.2568 (14)	C1—H1A	0.970
Ag1—Cl1^{i}	2.3117 (11)	C1—H1B	0.970
K1—O2	2.783 (2)	C2—C3	1.484 (4)
K1—O2^{ii}	2.783 (2)	C2—H2A	0.970
K1—O3^{ii}	2.8145 (19)	C2—H2B	0.970
K1—O3	2.8145 (19)	C3—H3A	0.970
K1—O1^{ii}	2.830 (2)	C3—H3B	0.970
K1—O1	2.830 (2)	C4—C5	1.471 (5)
K1—Cl1^{ii}	3.2568 (14)	C4—H4A	0.970
O1—C2	1.409 (4)	C4—H4B	0.970
O1—C1	1.430 (4)	C5—H5A	0.970
O2—C4	1.405 (4)	C5—H5B	0.970
O2—C3	1.413 (3)	C6—C1^{ii}	1.477 (4)
O3—C6	1.415 (3)	C6—H6A	0.970
O3—C5	1.419 (3)	C6—H6B	0.970
Ag1—Cl1—K1	93.96 (4)	C5—O3—K1	112.68 (16)
Cl1^{i}—Ag1—Cl1	180.0	O1—C1—C6^{ii}	109.6 (3)
O2—K1—O2^{ii}	180.0	O1—C1—H1A	109.7
O2—K1—O3^{ii}	120.16 (6)	C6^{ii}—C1—H1A	109.7
O2^{ii}—K1—O3^{ii}	59.84 (6)	O1—C1—H1B	109.7
O2—K1—O3	59.84 (6)	C6^{ii}—C1—H1B	109.7
O2^{ii}—K1—O3	120.16 (6)	H1A—C1—H1B	108.2
O3^{ii}—K1—O3	180.0	O1—C2—C3	109.4 (2)
O2—K1—O1^{ii}	119.12 (6)	O1—C2—H2A	109.8
O2^{ii}—K1—O1^{ii}	60.88 (6)	C3—C2—H2A	109.8
O3^{ii}—K1—O1^{ii}	119.26 (6)	O1—C2—H2B	109.8
O3—K1—O1^{ii}	60.74 (6)	C3—C2—H2B	109.8
O2—K1—O1	60.88 (6)	H2A—C2—H2B	108.2
O2^{ii}—K1—O1	119.12 (6)	O2—C3—C2	108.2 (2)
O3^{ii}—K1—O1	60.74 (6)	O2—C3—H3A	110.1
O3—K1—O1	119.26 (6)	C2—C3—H3A	110.1
O1^{ii}—K1—O1	180.0	O2—C3—H3B	110.1

O2—K1—Cl1^{ii}	104.35 (5)	C2—C3—H3B	110.1
O2^{ii}—K1—Cl1^{ii}	75.65 (5)	H3A—C3—H3B	108.4
O3^{ii}—K1—Cl1^{ii}	96.71 (5)	O2—C4—C5	108.6 (3)
O3—K1—Cl1^{ii}	83.29 (5)	O2—C4—H4A	110.0
O1^{ii}—K1—Cl1^{ii}	80.62 (4)	C5—C4—H4A	110.0
O1—K1—Cl1^{ii}	99.38 (4)	O2—C4—H4B	110.0
O2—K1—Cl1	75.65 (5)	C5—C4—H4B	110.0
O2^{ii}—K1—Cl1	104.35 (5)	H4A—C4—H4B	108.4
O3^{ii}—K1—Cl1	83.29 (5)	O3—C5—C4	109.9 (3)
O3—K1—Cl1	96.71 (5)	O3—C5—H5A	109.7
O1^{ii}—K1—Cl1	99.38 (4)	C4—C5—H5A	109.7
O1—K1—Cl1	80.62 (4)	O3—C5—H5B	109.7
Cl1^{ii}—K1—Cl1	180.0	C4—C5—H5B	109.7
C2—O1—C1	112.0 (2)	H5A—C5—H5B	108.2
C2—O1—K1	110.46 (17)	O3—C6—C1^{ii}	108.9 (3)
C1—O1—K1	110.70 (17)	O3—C6—H6A	109.9
C4—O2—C3	114.2 (2)	C1^{ii}—C6—H6A	109.9
C4—O2—K1	116.99 (17)	O3—C6—H6B	109.9
C3—O2—K1	114.25 (16)	C1^{ii}—C6—H6B	109.9
C6—O3—C5	113.9 (3)	H6A—C6—H6B	108.3
C6—O3—K1	114.53 (18)		
Ag1—Cl1—K1—O2	176.84 (5)	Cl1^{ii}—K1—O2—C3	−77.49 (18)
Ag1—Cl1—K1—O2^{ii}	−3.16 (5)	Cl1—K1—O2—C3	102.51 (18)
Ag1—Cl1—K1—O3^{ii}	−59.64 (5)	O2—K1—O3—C6	−152.6 (2)
Ag1—Cl1—K1—O3	120.36 (5)	O2^{ii}—K1—O3—C6	27.4 (2)
Ag1—Cl1—K1—O1^{ii}	59.01 (5)	O1^{ii}—K1—O3—C6	13.5 (2)
Ag1—Cl1—K1—O1	−120.99 (5)	O1—K1—O3—C6	−166.5 (2)
O2—K1—O1—C2	20.34 (18)	Cl1^{ii}—K1—O3—C6	96.4 (2)
O2^{ii}—K1—O1—C2	−159.66 (18)	Cl1—K1—O3—C6	−83.6 (2)
O3^{ii}—K1—O1—C2	−145.9 (2)	O2—K1—O3—C5	−20.37 (19)
O3—K1—O1—C2	34.1 (2)	O2^{ii}—K1—O3—C5	159.63 (19)
Cl1^{ii}—K1—O1—C2	121.62 (18)	O1^{ii}—K1—O3—C5	145.7 (2)
Cl1—K1—O1—C2	−58.38 (18)	O1—K1—O3—C5	−34.3 (2)
O2—K1—O1—C1	145.0 (2)	Cl1^{ii}—K1—O3—C5	−131.3 (2)
O2^{ii}—K1—O1—C1	−35.0 (2)	Cl1—K1—O3—C5	48.7 (2)
O3^{ii}—K1—O1—C1	−21.23 (18)	C2—O1—C1—C6^{ii}	178.3 (3)
O3—K1—O1—C1	158.77 (18)	K1—O1—C1—C6^{ii}	54.5 (3)
Cl1^{ii}—K1—O1—C1	−113.71 (19)	C1—O1—C2—C3	−177.8 (2)
Cl1—K1—O1—C1	66.29 (19)	K1—O1—C2—C3	−53.9 (3)
O3^{ii}—K1—O2—C4	166.4 (2)	C4—O2—C3—C2	173.3 (2)
O3—K1—O2—C4	−13.6 (2)	K1—O2—C3—C2	−48.3 (3)
O1^{ii}—K1—O2—C4	−27.5 (2)	O1—C2—C3—O2	70.3 (3)
O1—K1—O2—C4	152.5 (2)	C3—O2—C4—C5	−178.1 (2)

Cl1^{ii}—K1—O2—C4	59.7 (2)	K1—O2—C4—C5	44.7 (3)
Cl1—K1—O2—C4	−120.3 (2)	C6—O3—C5—C4	−175.2 (3)
O3^{ii}—K1—O2—C3	29.3 (2)	K1—O3—C5—C4	52.2 (3)
O3—K1—O2—C3	−150.7 (2)	O2—C4—C5—O3	−64.7 (3)
O1^{ii}—K1—O2—C3	−164.62 (17)	C5—O3—C6—C1^{ii}	−177.8 (3)
O1—K1—O2—C3	15.38 (17)	K1—O3—C6—C1^{ii}	−46.1 (3)

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

Fig. 1

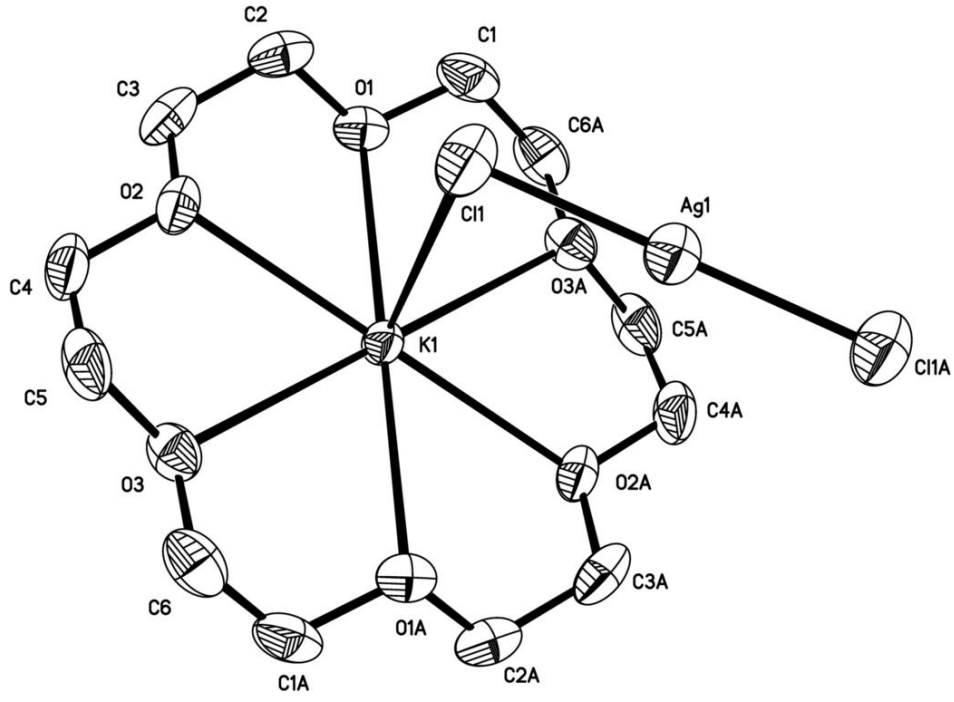
C2
C1
C3
O1
C6A
O2
Cl1
Ag1
C4
O3A
C5A
K1
Cl1A
C5
C4A
O3
O2A
C3A
C6
O1A
C1A
C2A

Fig. 2