S1—C2	1.812 (7)	O13—C14	1.432 (10)
S1—C18	1.819 (7)	C14—C15	1.502 (12)
C2—C3	1.520 (10)	C15—O16	1.429 (9)
C3—S4	1.809 (7)	O16—C17	1.411 (9)
S4—C5	1.814 (7)	C17—C18	1.510 (11)
C5—C6	1.507 (10)		
Cl11—Hg1—Cl12	109.43 (7)	C3—S4—C5	104.6 (3)
Cl12—Hg1—S4	136.22 (6)	C6—C5—S4	112.6 (5)
Cl11—Hg1—S4	106.40 (7)	O7—C6—C5	107.6 (6)
Cl12—Hg1—S1	100.42 (7)	C6—O7—C8	113.5 (6)
Cl11—Hg1—S1	115.19 (7)	O7—C8—C9	107.5 (6)
S1—Hg1—S4	86.06 (6)	O10—C9—C8	110.3 (6)
Cl22—Hg2—Cl21	166.90 (7)	C9—O10—C11	111.0 (6)
Cl22—Hg2—Cl12	95.87 (7)	O10—C11—C12	110.1 (6)
Cl21—Hg2—Cl12	94.86 (7)	O13—C12—C11	110.4 (7)
Hg1—Cl12—Hg2	96.07 (7)	C12—O13—C14	110.4 (6)
C2—S1—C18	104.6 (3)	O13—C14—C15	109.8 (7)
Hg1—S1—C2	96.9 (2)	O16—C15—C14	108.3 (6)
C18—S1—Hg1	101.4 (3)	C17—O16—C15	112.8 (6)
S1—C2—C3	115.3 (5)	O16—C17—C18	108.7 (6)
C2—C3—S4	117.1 (5)	C17—C18—S1	112.7 (5)
C18—S1—C2—C3	61.8 (6)	C9—O10—C11—C12	173.5 (6)
S1—C2—C3—S4	61.5 (7)	O10—C11—C12—O13	−70.0 (8)
C2—C3—S4—C5	62.9 (6)	C11—C12—O13—C14	−172.0 (7)
C3—S4—C5—C6	76.9 (6)	C12—O13—C14—C15	−174.3 (7)
S4—C5—C6—O7	−66.8 (7)	O13—C14—C15—O16	70.0 (9)
C5—C6—O7—C8	168.5 (6)	C14—C15—O16—C17	173.2 (6)
C6—O7—C8—C9	179.1 (6)	C15—O16—C17—C18	162.9 (6)
O7—C8—C9—O10	60.4 (8)	O16—C17—C18—S1	−78.7 (7)
C8—C9—O10—C11	176.9 (6)	C2—S1—C18—C17	61.4 (6)

Data collection: *DIF*4 (Stoe & Cie, 1990*a*). Cell refinement: *DIF*4. Data reduction: *REDU*4 (Stoe & Cie, 1990*b*). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *SHELXTL/PC* (Sheldrick, 1992). Software used to prepare material for publication: *SHELXL*93.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: CF1033). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Potassium Dibenzo-18-crown-6 Triiodide

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Abstract

In (1,4,7,10,13,16-hexaoxa-2,3:11,12-dibenzocyclooctadeca-2,11-diene)potassium triiodide, $[K(C_{20}H_{24}O_6)]I_3$, the K^+ ion is coordinated to the six ether O donors of the macrocycle [K—O 2.716 (4)–2.779 (4) Å] and to atom I3 at a distance of 3.6002 (13) Å; I1—I2 is 2.8741 (7) and I2—I3 2.9838 (7) Å. Pairs of symmetry-related [K(dibenzo-18-crown-6)]I_3 molecules aggregate, with an unusually short distance of 3.184 (3) Å between the K^+ ion and the centroid of one of the benzo groups.

Comment

We are interested in the stabilization of extended polyiodide networks by metal macrocyclic complexes and our work has focused on complexes containing homoleptic S-donor macrocycles (Blake, Devillanova, Lippolis & Schröder, 1994; Blake, Gould, Parsons, Radek & Schröder, 1995).

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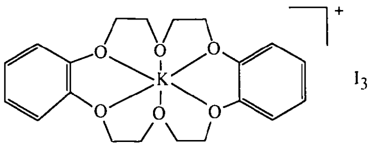
The structure of $[K(2,2\text{-Crypt})]I_3$ (2,2-Crypt = 1,4,10,13-tetraoxa-7,16-diazacyclooctadecane) has been reported (Tebbe & Kavoosian, 1995) and features a one-dimensional network formed by zigzag chains of alternating bridging I_3^- anions and $[K(2,2\text{-Crypt})]^+$ cations. We are interested in establishing whether complexes between triiodide and homoleptic O-donor macrocycles show similar features and we report herein the synthesis and single-crystal X-ray structure of the metal macrocyclic complex $[K(\text{dibenzo-18-crown-6})]I_3$, (1).



(1)

The asymmetric unit in the crystal structure of (1) shows features typical of complexes containing the $[K(\text{dibenzo-18-crown-6})]^+$ moiety (Fig. 1). The K^+ ion lies near the centre of the macrocyclic cavity [K—O 2.716 (4)–2.779 (4) Å], but is displaced by 0.273 (2) Å from the O_6 mean plane in the direction away from I3; the O atoms deviate from the O_6 mean plane by up to 0.104 (3) Å. Within the crown ether the aliphatic C—C, aromatic C—C and C—O distances average 1.506 (8), 1.388 (8) and 1.413 (7) Å, respectively, in agreement with corresponding values in other complexes (Mok & McKee, 1990). The K^+ ion shows an additional long-range interaction with the terminal I3 atom [K$\cdots$I3 3.6002 (13) Å] of the asymmetric I_3^- anion [I1—I2 2.8741 (7) and I2—I3 2.9838 (7) Å]. The triiodide anion is aligned approximately parallel to the major inertial axis of the $[K(\text{dibenzo-18-crown-6})]^+$ cation and the other terminal I atom (I1) lies directly above the centroid *B* of the benzo group (C15–C20, Fig. 1) at a distance of 4.332 (9) Å.

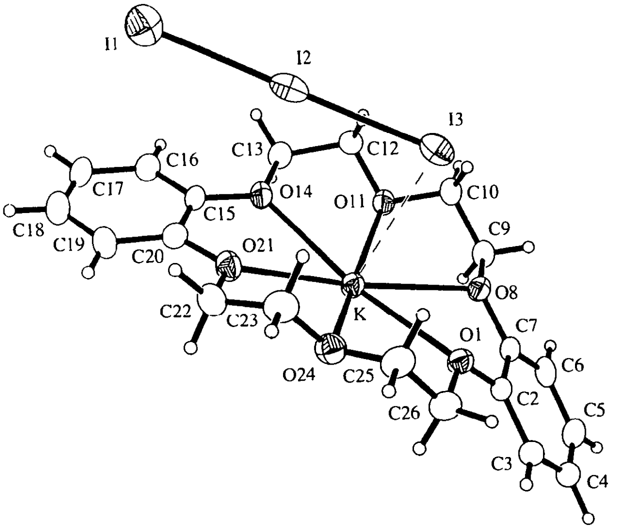


Fig. 1. A view of the contents of the asymmetric unit of (1) showing the atom-numbering scheme. Displacement ellipsoids enclose 50% probability surfaces and H atoms are drawn as spheres of arbitrary radii.

Fig. 2 shows two symmetry-related formula units (at x, y, z and $-1-x, -y, 1-z$) in close proximity; there is an unusually short distance of 3.184 (3) Å between the centroid *B* and the K^+ ion, with an $I_3^-\cdots K^+\cdots B$ angle of 173.80 (8)°.

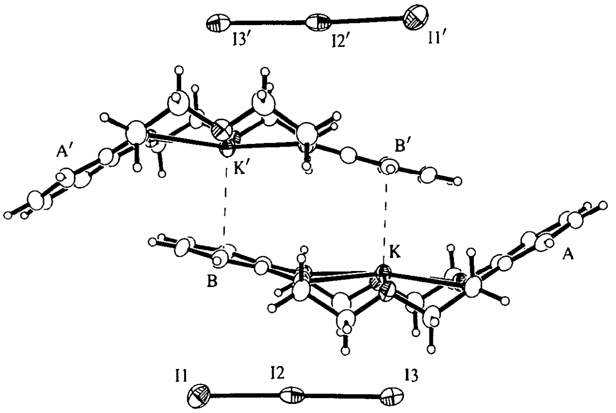


Fig. 2. A view illustrating the aggregation of two formula units. Dashed lines between K^+ and the centroid *B* indicate distances of 3.184 (3) Å and dotted lines between K^+ and I_3 indicate distances of 3.6002 (13) Å.

Interactions between the $[K(\text{dibenzo-18-crown-6})]^+$ cation and aromatic rings have been reported for other compounds. However, these interactions were between the $[K(\text{dibenzo-18-crown-6})]^+$ moiety and molecules such as benzene (Hrncir, Rodgers & Atwood, 1981; Atwood, Hrncir & Rodgers, 1983) or naphthalene (Atwood, Hunter, Rodgers & Weeks, 1985) trapped in the crystal lattice. The distances between K^+ and the centroids of the aromatic rings in these compounds are similar [3.369, 3.119 and 3.344 Å, respectively] to those in (1). They also show a quasi-linear interaction involving the centroid of the aromatic ring, the K^+ ion and the seventh coordinated species. We are presently pursuing the structures of analogous complexes involving 18-crown-6 and 15-crown-5.

Experimental

Dibenzo-18-crown-6 was freshly recrystallized from refluxing EtOH. KI and I_2 were added to a solution of dibenzo-18-crown-6 in MeCN. Slow evaporation afforded single crystals of (1) suitable for X-ray diffraction studies. Microanalysis for $C_{20}H_{24}I_3KO_6$: calculated C 30.79, H 3.10%; found C 30.99, H 2.97%. Fast-atom bombardment (FAB) mass spectrum (glycerol/thioglycerol) *m*/*z*: 399; calculated for $[K(C_{20}H_{24}O_6)]^+$ 399.

Crystal data

$[K(C_{20}H_{24}O_6)]I_3$
$M_r = 780.19$
Monoclinic
$P2_1/n$
$a = 9.7749\,(14)$ Å
$b = 16.821\,(3)$ Å
$c = 15.293\,(2)$ Å
$\beta = 99.501\,(14)°$
$V = 2480.0\,(7)$ Å^3
$Z = 4$
$D_x = 2.090$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 84 reflections
$\theta = 15\text{–}16°$
$\mu = 3.981$ mm^{-1}
$T = 150.0\,(2)$ K
Block
$0.58 \times 0.39 \times 0.39$ mm
Red

Data collection

Stoe Stadi-4 four-circle diffractometer
ω–2θ scans
Absorption correction:
ψ scans
$T_{\min} = 0.068$, $T_{\max} = 0.094$
5958 measured reflections
4362 independent reflections

3687 observed reflections $[I > 2\sigma(I)]$
$R_{\text{int}} = 0.0747$
$\theta_{\max} = 25.04°$
$h = -11 \rightarrow 11$
$k = -5 \rightarrow 19$
$l = 0 \rightarrow 18$
3 standard reflections
frequency: 60 min
intensity decay: 2%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.0419$
$wR(F^2) = 0.1159$
$S = 1.046$
4350 reflections
272 parameters
$w = 1/[\sigma^2(F_o^2) + (0.073P)^2 + 1.47P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = -0.16$
$\Delta\rho_{\max} = 0.98$ e Å^{-3}
$\Delta\rho_{\min} = -1.91$ e Å^{-3}

Extinction correction: *SHELXL*93 (Sheldrick, 1993)
Extinction coefficient: 0.0026 (3)
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$$U_{\text{eq}} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
I1	0.02148 (5)	0.23358 (3)	0.48950 (3)	0.0502 (2)
I2	−0.09192 (4)	0.20386 (2)	0.64824 (3)	0.0379 (2)
I3	−0.21122 (4)	0.18356 (2)	0.81430 (3)	0.0420 (2)
K	−0.46815 (11)	0.05926 (7)	0.68477 (7)	0.0267 (3)
O1	−0.6254 (3)	0.1291 (2)	0.7996 (2)	0.0273 (8)
C2	−0.6878 (5)	0.0772 (3)	0.8501 (3)	0.0278 (11)
C3	−0.8194 (5)	0.0871 (4)	0.8715 (3)	0.0360 (13)
C4	−0.8744 (5)	0.0291 (4)	0.9213 (3)	0.0392 (14)
C5	−0.7998 (6)	−0.0368 (4)	0.9488 (4)	0.0398 (14)
C6	−0.6660 (6)	−0.0478 (4)	0.9281 (3)	0.0340 (12)
C7	−0.6119 (5)	0.0089 (3)	0.8791 (3)	0.0242 (10)
O8	−0.4821 (3)	0.0032 (2)	0.8534 (2)	0.0268 (8)
C9	−0.4069 (5)	−0.0680 (3)	0.8755 (3)	0.0296 (11)
C10	−0.2694 (6)	−0.0608 (4)	0.8457 (3)	0.0318 (12)
O11	−0.2899 (4)	−0.0603 (2)	0.7508 (2)	0.0292 (8)
C12	−0.1596 (5)	−0.0498 (4)	0.7207 (3)	0.0316 (12)
C13	−0.1833 (5)	−0.0557 (3)	0.6208 (3)	0.0310 (12)
O14	−0.2745 (4)	0.0082 (2)	0.5861 (2)	0.0314 (8)
C15	−0.2788 (5)	0.0265 (3)	0.4987 (3)	0.0280 (11)
C16	−0.2085 (6)	−0.0134 (4)	0.4403 (4)	0.0348 (13)
C17	−0.2184 (6)	0.0134 (4)	0.3534 (4)	0.0396 (14)
C18	−0.2981 (6)	0.0780 (4)	0.3240 (4)	0.0410 (15)
C19	−0.3728 (6)	0.1169 (4)	0.3807 (3)	0.0385 (14)
C20	−0.3612 (5)	0.0934 (3)	0.4687 (3)	0.0302 (11)
O21	−0.4252 (4)	0.1296 (2)	0.5317 (2)	0.0318 (8)
C22	−0.4904 (6)	0.2059 (4)	0.5083 (4)	0.0387 (14)
C23	−0.5060 (6)	0.2488 (4)	0.5911 (4)	0.0388 (13)
O24	−0.5898 (4)	0.2030 (2)	0.6403 (2)	0.0340 (9)
C25	−0.6154 (6)	0.2468 (4)	0.7161 (4)	0.0370 (13)
C26	−0.7050 (6)	0.1965 (3)	0.7657 (4)	0.0357 (13)

Table 2. *Selected geometric parameters* (Å, °)

I1—I2	2.8741 (7)	K—O11	2.742 (4)
I2—I3	2.9838 (7)	K—O14	2.746 (4)
I3· · ·K	3.6002 (13)	K—O8	2.771 (3)
K—O21	2.716 (4)	K—O1	2.779 (4)
K—O24	2.730 (4)		
I1—I2—I3	176.55 (2)	O24—K—O8	116.55 (11)
I2—I3· · ·K	86.18 (2)	O11—K—O8	62.18 (10)
O21—K—O24	61.48 (12)	O14—K—O8	123.33 (11)
O21—K—O11	117.24 (11)	O21—K—O1	122.73 (12)
O24—K—O11	164.86 (12)	O24—K—O1	61.27 (11)
O21—K—O14	56.23 (11)	O11—K—O1	117.48 (11)
O24—K—O14	116.83 (12)	O14—K—O1	169.47 (12)
O11—K—O14	61.28 (11)	O8—K—O1	55.81 (10)
O21—K—O8	171.39 (11)		

The crystal was mounted on a glass fibre and placed in the nitrogen stream of an Oxford Cryosystems low-temperature device (Cosier & Glazer, 1986). All methylene H atoms were allowed to ride on their parent atoms with C—H = 0.99 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The remaining H atoms were refined riding on idealized hexagons with C—H = 0.95 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: *DIF*4 (Stoe & Cie, 1990*a*). Cell refinement: *DIF*4. Data reduction: *REDU*4 (Stoe & Cie, 1990*b*). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *SHELXTL*/*PC* (Sheldrick, 1992). Software used to prepare material for publication: *SHELXL*93.

We thank the SERC for support.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: HA1143). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Acta Cryst. (1996). C52, 27–29

The Heterotrimetallic Linear Complex Tetraethylammonium Dibromo-2κ^2*Br*-tetra-μ-sulfido-1:2κ^4*S*;1:3κ^4*S*-bis(triphenylphosphine-3κ*P*)-2-iron-3-silver-1-tungsten, $[Et_4N][Br_2FeS_2WS_2Ag(PPh_3)_2]$

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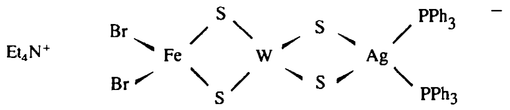
(*Received 27 March 1995; accepted 18 July 1995*)

Abstract

The structure of the title complex, $(C_8H_{20}N)$-$[AgFeWS_4Br_2(C_{18}H_{15}P)_2]$, can be simply described as linear with three types of metal atoms distributed along a line. Each metal atom is approximately tetrahedrally coordinated.

Comment

Syntheses of heterotrimetallic compounds are still challenging (Richter & Vahrenkamp, 1978; Gheller *et al.*, 1984; Planalp & Vahrenkamp, 1987). Recently, a few heterotrimetallic complexes have been designedly synthesized in our laboratory, such as the butterfly-like complexes $[Et_4N][(PPh_3)_2AgO\mathit{M}S_3CuCN]$ and the linear complexes $[Et_4N][Cl_2FeS_2\mathit{M}S_2\mathit{M}'(PPh_3)_2]$ and $[Et_4N][(PPh_3)_2AgS_2\mathit{M}S_2CuCN]$ (M = Mo, W; M' = Cu, Ag) (Du, Zhu, Chen, Wu & Lu, 1992*a*,*b*; Zhu, Du, Chen & Wu, 1992; Sheng, Du & Wu, 1993*a*,*b*). The structure of $[Et_4N][Br_2FeS_2WS_2Ag(PPh_3)_2]$, (I), was studied as a supplementary member of the family of heterotrimetallic linear complexes $\{FeS_2\mathit{M}S_2\mathit{M}'\}$ (M = Mo, W; M' = Cu, Ag).



(I)

The Ag···W···Fe angle of 177.04 (3)° suggests that the arrangement of the three metal atoms is essentially linear. The WS_2Ag and WS_2Fe fragments are planar, forming a dihedral angle of 90.07 (5)° between their planes; *i.e.* these two fragments are almost perpendicular to each other. The W atom is coordinated by four μ_2-S atoms with approximate tetrahedral geometry [106.79 (9)–113.12 (9)°]. However, two μ_2-S and two Br atoms about the Fe atom are arranged with slightly distorted tetrahedral geometry [102.06 (9)–112.6 (1)°], and two μ_2-S and two P atoms about the Ag atom with severely distorted tetrahedral geometry [88.56 (7)–118.27 (7)°]. One reason for the distortions of the tetrahedral geometries about Fe and Ag is the differences in the M—S bond lengths [mean W—S, Ag—S and Fe—S lengths 2.210 (2), 2.616 (2) and 2.304 (3) Å, respectively]; the longer Ag—S distance results in a smaller S—Ag—S angle. The W—Ag and W—Fe distances are 3.0788 (7) and 2.779 (1) Å, respectively, which are similar to the corresponding values found in $[Et_4N][Cl_2FeS_2WS_2Ag(PPh_3)_2]$ [3.076 (1) and 2.786 (2) Å, respectively]. The title complex and $[Et_4N][Cl_2FeS_2WS_2Ag(PPh_3)_2]$ are isomorphic.

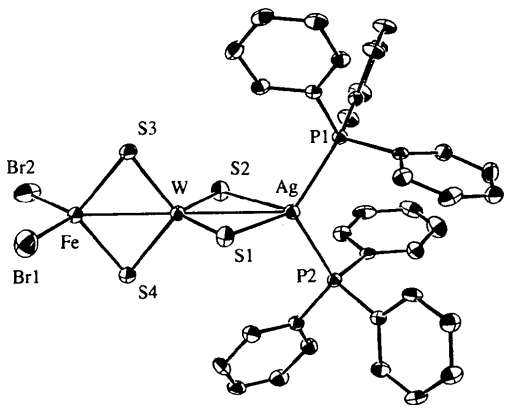


Fig. 1. Structure of the anion showing 20% probability displacement ellipsoids. C atoms are unlabelled for clarity.

Experimental

The complex was synthesized under nitrogen atmosphere by reaction of $[Et_4N][S_2WS_2FeBr_2]$ and $Ag(PPh_3)_3I$ (molar ratio 1:1) in CH_3CN and CH_2Cl_2, and crystallized by slow diffusion of Et_2O into the filtrate.

Crystal data

$(C_8H_{20}N)[AgFeWS_4Br_2$-$(C_{18}H_{15}P)_2]$
M_r = 1290.48
Triclinic
$P\bar{1}$
a = 13.527 (4) Å
b = 15.592 (5) Å
c = 12.429 (6) Å
α = 104.91 (3)°
β = 94.72 (3)°
γ = 101.19 (2)°
V = 2460.8 Å^3
Z = 2
D_x = 1.74 Mg m^{-3}

Mo $K\alpha$ radiation
λ = 0.71073 Å
Cell parameters from 20 reflections
θ = 3–12.5°
μ = 4.93 mm^{-1}
T = 296 K
Rectangular
0.80 × 0.60 × 0.30 mm
Dark red