to 104·7° for $[Mo_2Cl_8]^{4-}$. The mean S—Cl distance between the eclipsed ligands is 3·29 (5) Å which is quite comparable to the 3·38 (2) Å Cl—Cl distance in $[Mo_2Cl_8]^{4-}$.

The structure reported here is probably typical for all of the monodentate sulfide and phosphine compounds of formula $Mo_2X_4L_4$. These compounds are all dark blue and have nearly identical electronic spectra and physical properties. Attempts to obtain crystals of the presumed chelated complexes of the blue-green bidentate sulfides were unsuccessful.

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The Structure of Rubidium Hydrogen Bis(dibromoacetate)

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Abstract. $RbH(C_2HBr_2O_2)_2$, $Rb^+.C_4H_3Br_4O_4^-$, FW = 520·15, monoclinic, $P2_1/n$, a = 6·299 (3), b = 20·958 (5), c = 4·446 (3) Å, β = 98·05 (3)°, V = 581·2 Å^3, Z = 2, μ = 19·04 mm^{-1}, λ(Mo $K\alpha$), D_c = 2·98 Mg m^{-3}. Final R = 0·074 for 741 reflections with $I \geq 1·92\ \sigma(I)$. The crystal has a layer structure. Within the layers [parallel to the (010) plane] the hydrogen bis(dibromoacetate) anions are connected by Rb^+ cations. The two dibromoacetate residues are linked by a symmetric ($\bar{1}$) hydrogen bond with O···O = 2·43 (2) Å.

Introduction. We have determined the crystal structures of caesium (Głowiak, Videnova, Baran & Ratajczak, 1980) and potassium hydrogen bis(dibromoacetate) (Baran, Videnova, Głowiak & Ratajczak, 1979). In these crystals strong hydrogen bonds between two dibromoacetate residues are present with O···O = 2·50 (2) and 2·44 (3) Å respectively. Now we report the crystal structure of the title compound.

Crystals of $RbH(C_2HBr_2O_2)_2$ were prepared by adding dibromoacetic acid to Rb_2CO_3 in 4:1 molar ratio in an excess of H_2O. The solution was then evaporated to form colourless crystals.

The cell dimensions and intensities were measured on a Syntex $P2_1$ four-circle diffractometer with a graphite monochromator and Mo $K\alpha$ radiation. The lattice parameters and orientation matrix used for data collection were obtained by least squares from 15 reflections. Intensities of 1081 reflections were collected by the θ–2θ scan technique to $2\theta = 60°$. 741 reflections with $I \geq 1·92\sigma(I)$ were accepted for further calculations. Standard reflections were measured every 15 reflections and showed no significant change. The data were corrected for Lorentz and polarization factors, but not for absorption. The structure was solved by the heavy-atom technique. The positions of all non-H atoms were found from a Patterson synthesis and from difference maps. The positions of the H atoms were not found. The refinement gave R_1 = 0·087 and R_2 = 0·072. The function minimized during refinement was $\sum w(|F_o| - |F_c|)^2$ with $w = 1/\sigma^2(F)$. Scattering factors were taken from *International Tables for X-ray*

Table 1. *The atomic coordinates* (×10^4) *with e.s.d.'s in parentheses*

	x	y	z
Rb	0	0	0
Br(1)	3209 (4)	3598 (1)	577 (6)
Br(2)	−1058 (5)	2967 (1)	2161 (6)
O(1)	596 (25)	4494 (6)	4071 (30)
O(2)	−2281 (28)	4516 (7)	488 (34)
C(1)	−597 (40)	4292 (10)	1690 (54)
C(2)	201 (36)	3662 (9)	138 (46)

Symmetry code

(i)	0·00 + x,	0·00 + y,	0·00 + z
(ii)	0·50 − x,	0·50 + y,	0·50 − z
(iii)	0·00 − x,	0·00 − y,	0·00 − z
(iv)	−0·50 + x,	−0·50 − y,	−0·50 + z

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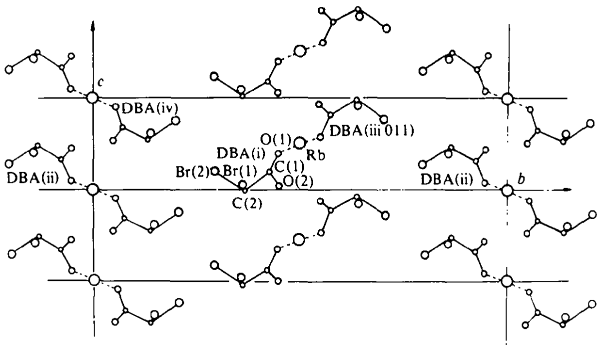

Fig. 1. Projection of the structure on the *bc* plane.

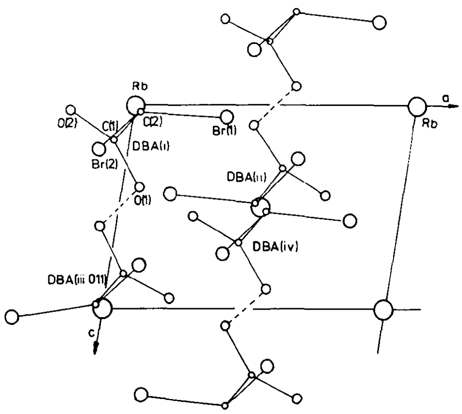

Fig. 2. Projection of the structure on the *ac* plane.

Crystallography (1974). All calculations were carried out on a Nova minicomputer with programs supplied by Syntex.

Final atomic parameters are given in Table 1.*

Discussion. A general impression of the crystal structure can be obtained from Figs. 1 and 2. Rubidium hydrogen bis(dibromoacetate) has a layer structure. The layers are parallel to the (010) crystallographic plane and are built from dimeric anions $H(C_2HBr_2O_2)_2^-$ and Rb^+ cations both of which are in positions of $\bar{1}$ symmetry. The Rb^+ cation makes contact with eight O atoms, which belong to eight different dibromoacetate residues, and with two Br(1) atoms (Table 2). The Rb^+ cations interact with four O(2) and four O(1) atoms. Each O atom interacts with two Rb^+ cations. The $Rb^+\cdots O(2)$ distances are 2·957 (16) and 2·991 (16) Å and all O(2) atoms are in contact with one pair of Rb^+ cations related by a *c* translation. The $Rb^+\cdots O(1)$ distances are 2·944 (16) and 3·759 (16) Å and all O(1) atoms contact one pair of Rb^+ cations related by an *a* translation. The $Rb^+\cdots Br(1)$ distances are 3·625 (3) Å. Thus the dibromoacetic acid residues are connected to three different Rb^+ cations through O(1), O(2) and Br(1).

Two adjacent layers are connected through the Br atoms. The shortest distance between Br atoms belonging to adjacent layers is 3·672 (4) Å, Br(1)$\cdots$Br(2^{iv110}).

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 34876 (23 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *The environment of the* Rb^+ *cations*

Rb–O(1^a)	2·944 (16) Å	Rb–O(2^f)	2·957 (16) Å
Rb–O(1^b)	2·944 (16)	Rb–O(1^d)	3·759 (16)
Rb–O(2^c)	2·991 (16)	Rb–O(1^c)	3·759 (16)
Rb–O(2^d)	2·991 (16)	Rb–Br(1^a)	3·625 (3)
Rb–O(2^e)	2·957 (16)	Rb–Br(1^b)	3·625 (3)

Br(1^a)–Rb–O(2^f)	74·3 (3)°	O(1^a)–Rb–O(2^c)	113·6 (4)°
Br(1^a)–Rb–O(2^e)	105·6 (3)	O(1^a)–Rb–O(1^b)	180·0 (4)
Br(1^a)–Rb–O(2^d)	118·3 (3)	O(2^c)–Rb–O(2^f)	83·2 (4)
Br(1^a)–Rb–O(2^c)	61·6 (3)	O(2^c)–Rb–O(2^e)	96·7 (4)
Br(1^a)–Rb–O(1^b)	125·6 (3)	O(1^d)–Rb–O(2^f)	63·2 (4)
Br(1^a)–Rb–O(1^d)	54·3 (3)	O(1^d)–Rb–O(2^e)	116·7 (4)
O(1^a)–Rb–O(2^f)	65·3 (4)	O(1^d)–Rb–O(2^d)	36·5 (4)
O(1^a)–Rb–O(2^e)	114·7 (4)	O(1^d)–Rb–O(2^c)	143·4 (4)
O(1^a)–Rb–O(2^d)	66·3 (4)	O(1^c)–Rb–O(1^b)	40·2 (4)

Symmetry code

(*a*)	$0.50-x$,	$-0.50+y$,	$0.50-z$
(*b*)	$-0.50+x$,	$0.50-y$,	$-0.50+z$
(*c*)	$-0.50-x$,	$-0.50+y$,	$0.50-z$
(*d*)	$0.50-x$,	$0.50-y$,	$-0.50+z$
(*e*)	$-0.50-x$,	$-0.50+y$,	$-0.50-z$
(*f*)	$0.50+x$,	$0.50-y$,	$0.50+z$

Table 3. *The molecular plane for the* $RbH(C_2HBr_2O_2)_2$ *crystal*

Plane through O(1), O(2), C(1), C(2)

$$0.5873X + 0.5696Y - 0.5750Z - 4.4077 = 0$$

Distances of atoms from the plane (Å)

Rb	−4·4077
Br(1)	0·909 (3)
Br(2)	−1·883 (3)

Table 4. *Interatomic distances* (Å) *and angles* (°) *in the dibromoacetate residue with e.s.d.'s in parentheses*

C(1)–O(1)	1·28 (3)	O(1)–C(1)–O(2)	127·7 (22)
C(1)–O(2)	1·21 (3)	O(1)–C(1)–C(2)	116·4 (19)
C(1)–C(2)	1·60 (3)	O(2)–C(1)–C(2)	115·9 (20)
C(2)–Br(1)	1·88 (2)	C(1)–C(2)–Br(1)	112·7 (14)
C(2)–Br(2)	1·94 (2)	C(1)–C(2)–Br(2)	104·2 (14)
Br(1)–Br(2)	3·163 (4)	Br(2)–C(2)–Br(1)	111·7 (10)
O(1)–O(2)	2·24 (2)		

The two crystallographically equivalent dibromoacetate residues are bonded by a strong symmetric ($\bar{1}$) hydrogen bond with O(1)···O(1^{iii011}) = 2·43 (2) Å. The C and O atoms of the dimeric anions are virtually coplanar (Table 3) with maximum deviations from the plane less than standard errors.

The interatomic distances and angles of each dibromoacetate residue (Table 4) do not differ significantly from the corresponding bonds in the other acid salts of type *A* in the Speakman (1972) classification. The C–Br bond lengths [1·88 (2), 1·94 (2) Å] are similar to those in caesium and potassium hydrogen bis(dibromoacetate) (Głowiak, Videnova, Baran & Ratajczak, 1980; Baran, Videnova, Głowiak & Ratajczak, 1979).

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