Crystal and Molecular Structure of Tetra-μ-*o*-bromobenzoato-bis[aquo-copper(II)]

By **W. Harrison, S. Rettig,** and **J. Trotter,*** Department of Chemistry, University of British Columbia, Vancouver 8, British Columbia, Canada

Crystals of the title compound are monoclinic, a = 7·384(6), b = 20·02(2), c = 11·04(1) Å, β = 105·4(1)° Z = 2, space group $P2_1/n$. The structure was determined by Patterson and Fourier syntheses, and refined by full-matrix least-square methods to R 0·099 for 985 observed reflexions. The crystal structure consists of centrosymmetric dimers, with four *o*-bromobenzoate anions forming *syn–syn* bridges between the pairs of copper atoms. Cu–Cu is 2·624(7), mean Cu–O(carboxylate) 1·99(3), and Cu–O(H_2O) 2·17(2) Å. Intermolecular hydrogen bonds (O · · · O 2·89 Å) are probably present.

A GREAT deal of effort has been made to determine the nature of the metal–metal interaction in copper(II) carboxylates.[1-5] Structural studies have shown that several of the copper(II) carboxylates form *syn–syn* [6] bridged dimers with Cu–Cu distances ranging from 2·6—2·7 Å,[7-16] while others are polymeric in the solid state.[17-19] The copper(II) carboxylates and their mono-adduct derivatives have anomalous magnetic properties which can be interpreted in terms of exchange coupling between magnetically isolated pairs of copper(II) ions. Considerable interest lies in the mechanism of the exchange coupling, for which two models have been suggested: a direct metal–metal interaction,[4,20] and super-exchange *via* the carboxylate groups.[21,22] It is not yet completely understood which of these models is correct, or whether the mechanism is a combination of both.[15]

Some of the factors which determine the occurrence of dinuclear complexes and the degree of magnetic interaction between the copper atoms have been noted.[3,23-25] In the arylcarboxylates, the steric effect predominates, bulky *ortho*-substituents resulting in the formation of dinuclear complexes. When there are no steric effects, reduction of the charge on the copper ions is important. High σ electron density on the carboxylate oxygen atoms (as measured by the pK_a of the parent acid), and adducts which lower the residual charge on the copper ions make the formation of dinuclear complexes favourable. The magnetic properties of the copper(II) carboxylates depend on both the identity of the parent acid and the adduct, if one is present.

The magnetic properties of copper(II) *o*-bromobenzoate have been determined.[25] The copper(II) arylcarboxylates have been extensively studied (*e.g.* refs. 23—25), but the only structural information available is for copper(II) aspirinate.[13] The present study was undertaken to provide structural data which may aid in the understanding of the magnetic properties of the copper(II) carboxylates.

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EXPERIMENTAL

Crystals of tetra-μ-*o*-bromobenzoato-bis[aquocopper(II)] [25] are dark green and irregularly developed. The crystal chosen for study was a hexagonal plate, flattened along *b*, 0·1 × 0·2 × 0·2 mm. Unit-cell and space-group data were obtained from film and diffractometer measurements. The unit-cell parameters were refined by a least-squares treatment of $\sin^2\theta$ values for 17 reflexions measured on a diffractometer with Mo-K_α radiation.

Crystal Data.—$C_{28}H_{20}Br_4Cu_2O_{10}$, $M = 963{\cdot}18$, Monoclinic, $a = 7{\cdot}384(6)$, $b = 20{\cdot}02(2)$, $c = 11{\cdot}04(1)$ Å, $\beta = 105{\cdot}4(1)^\circ$, $U = 1573(2)$ Å^3, $D_m = 2{\cdot}06(2)$, $Z = 2$, $D_c = 2{\cdot}033(3)$, $F_0(000) = 932$, Mo-K_α radiation, $\lambda = 0{\cdot}71069$ Å, μ(Mo-K_α) = 69 cm^{-1}. Space group $P2_1/n$ (C^5_{2h}, No. 14) from absent spectra: $0k0$, $k \neq 2n$ and $h0l$, $h + l \neq 2n$.

Intensities were measured on a Datex-automated General Electric XRD 6 diffractometer, with a scintillation counter, Mo-K_α radiation (zirconium filter and pulse-height analyser), and a θ—2θ scan at 2° min^{-1} over a range of $(1{\cdot}80 + 0{\cdot}86 \tan\theta)$ degrees in 2θ, with background counts of 20 s being measured at each end of the scan. Data were measured to 2θ 45° (minimum interplanar spacing 0·93 Å). A check reflexion was monitored every 20 reflexions throughout the data collection; its intensity underwent variations of up to ±15% of its original value, the final value being slightly higher than the initial value. Lorentz and polarization corrections were applied, and the structure-factor amplitudes were derived. No absorption correction was made. Of the 2118 independent reflexions measured, 1133 had intensities $<3\sigma(I)$ above background where $\sigma^2(I) = S + B + (0{\cdot}03S)^2$, with S = scan count and B = background count. These reflexions were classified as unobserved.

Structure Analysis and Refinement.—The positions of the copper and bromine atoms were determined from a three-dimensional Patterson function. One cycle of full-matrix least-squares refinement of the positional parameters of the heavy atoms gave R 0·315, and a difference-Fourier synthesis revealed all the remaining atom positions excluding hydrogen. Two cycles of isotropic refinement gave R 0·143. The heavy atoms were then refined anisotropically and the oxygen and carbon atoms isotropically for two cycles resulting in R 0·123. An attempt to refine the oxygen and carbon atoms anisotropically resulted in non-positive definite temperature factors. Convergence was reached at R 0·099, for 985 observed reflexions.

The least-squares refinement was based on the minimization of $\Sigma w(F_o - F_c)^2$. The scattering factors of ref. 26 were used, corrections for anomalous dispersion being introduced for the copper and bromine atoms. The anisotropic temperature factors are β_{ij} in the expression:

$$f = f^\circ \exp(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + 2\beta_{12}hk + 2\beta_{13}hl + 2\beta_{23}kl)$$

where f° is the tabulated scattering factor and f is that corrected for thermal motion. The weighting scheme: $\sqrt{w} = 1$ if $|F_o| \leqslant 100$, $\sqrt{w} = 100/|F_o|$ if $|F_o| > 100$, and $\sqrt{w} = 0{\cdot}1$ for unobserved reflexions gave constant average values of $w(F_o - F_c)^2$ over ranges of $|F_o|$, and was employed in the final stages of refinement.

On the final cycle of refinement, no parameter shift was $>0{\cdot}16\sigma$. A final electron-density difference map showed fluctuations of up to $\pm1{\cdot}95$ eÅ^{-3}, and the hydrogen atoms could not be located. The final positional and thermal parameters are given in Table 1. Measured and calculated structure factors are listed in Supplementary Publication No. SUP 20420 (5 pp., 1 microfiche).*

TABLE 1

Final positional (fractional, ×10^4) and thermal parameters, with standard deviations in parentheses

Atom	*x*	*y*	*z*	B/Å^2
Br(1)	6181(5)	1033(2)	2848(4)	*
Br(2)	−0052(6)	−1926(2)	2841(4)	*
Cu	−1471(5)	−0159(2)	0394(2)	*
O(1)	0181(31)	0157(12)	2044(21)	3·55(48)
O(2)	2687(28)	0405(11)	1350(19)	2·88(45)
O(3)	−0231(29)	−1048(12)	0637(20)	3·25(46)
O(4)	2312(30)	−0783(12)	0036(21)	3·34(48)
O(5)	3786(30)	−0452(12)	1140(21)	3·45(48)
C(1)	1812(45)	0360(17)	2189(31)	2·77(67)
C(2)	2819(39)	0577(15)	3541(27)	1·99(58)
C(3)	4560(46)	0911(19)	3875(33)	3·51(74)
C(4)	5271(47)	1122(20)	5101(33)	3·54(75)
C(5)	4243(53)	1039(21)	6009(37)	4·44(83)
C(6)	2452(47)	0756(19)	5677(34)	3·67(76)
C(7)	1750(47)	0528(19)	4415(33)	3·54(75)
C(8)	1445(36)	−1179(15)	0576(26)	1·54(52)
C(9)	2371(41)	−1817(17)	1156(29)	2·56(62)
C(10)	1895(41)	−2160(16)	2075(29)	2·29(62)
C(11)	3037(44)	−2725(18)	2660(31)	3·13(69)
C(12)	4500(56)	−2961(22)	2230(38)	4·87(94)
C(13)	4944(53)	−2606(21)	1242(37)	4·44(88)
C(14)	3848(44)	−2041(17)	0642(31)	2·96(68)

* Anisotropic thermal parameters (Å^2 × 10^4)

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_2
Br(1)	417(21)	683(31)	570(27)	−205(21)	154(18)	−116(23)
Br(2)	556(26)	681(34)	701(31)	135(23)	279(22)	206(26)
Cu	183(18)	373(25)	225(20)	017(19)	−008(15)	003(20)

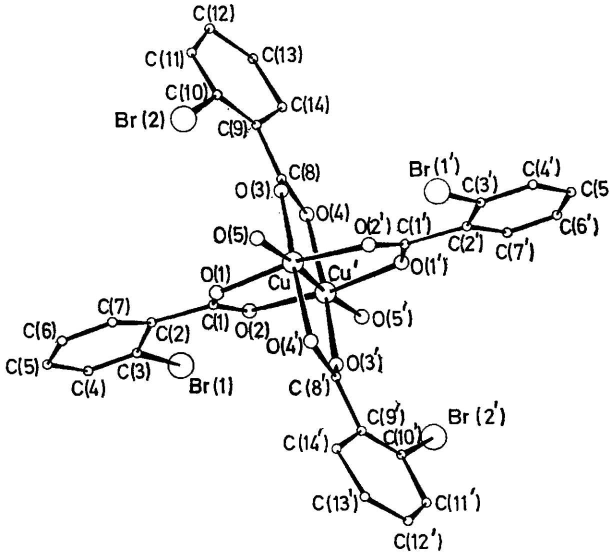

FIGURE 1 The $[Cu(o\text{-}BrC_6H_4CO_2)_2,H_2O]_2$ molecule viewed down *a*, showing the numbering scheme; primes refer to atoms related by the centre of symmetry to those in the asymmetric unit

DISCUSSION

Figure 1 shows the $[Cu(o\text{-}BrC_6H_4CO_2)_2(H_2O)]_2$ molecule viewed down *a*. Bond lengths and angles, with their

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* For details see Notice to Authors No. 7 in *J. Chem. Soc.* (*A*), 1970, Issue No. 20 (items less than 10 pp. are supplied as full size copies).

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TABLE 2

Bond lengths (Å), with standard deviations in parentheses *

Cu–Cu′	2·624(7)	C(1)–C(2)	1·54(4)
Cu–O(1)	2·01(2)	C(8)–C(9)	1·51(4)
Cu–O(2′)	1·96(2)	Mean	1·525(21)
Cu–O(3)	1·99(2)	C(2)–C(3)	1·41(4)
Cu–O(4′)	2·00(2)	C(3)–C(4)	1·38(5)
Mean	1·99(3)	C(4)–C(5)	1·42(5)
Cu–O(5)	2·17(2)	C(5)–C(6)	1·40(5)
C(1)–O(1)	1·24(4)	C(6)–C(7)	1·43(5)
C(1)–O(2)	1·27(3)	C(7)–C(2)	1·40(4)
C(8)–O(3)	1·28(3)	C(9)–C(10)	1·35(4)
C(8)–O(4)	1·26(3)	C(10)–C(11)	1·46(4)
Mean	1·26(2)	C(11)–C(12)	1·37(5)
C(3)–Br(1)	1·87(3)	C(12)–C(13)	1·41(5)
C(10)–Br(2)	1·91(3)	C(13)–C(14)	1·44(5)
Mean	1·89(2)	C(14)–C(9)	1·43(4)
		Mean	1·41(3)

* For the mean values, numbers in parentheses are root-mean-square deviations from the mean.

TABLE 3

Bond angles (°), standard deviations in parentheses

O(1)–Cu–O(2′)	169(1)	O(1)–C(1)–O(2)	127(3)
O(3)–Cu–O(4′)	168(1)	O(3)–C(8)–O(4)	121(3)
Mean	168·5(5)	Mean	124(3)
O(1)–Cu–O(3)	91(1)	O(1)–C(1)–C(2)	115(3)
O(1)–Cu–O(4′)	90(1)	O(2)–C(1)–C(2)	119(3)
O(2′)–Cu–O(3)	89(1)	O(3)–C(8)–C(9)	120(2)
O(2′)–Cu–O(4′)	88(1)	O(4)–C(8)–C(9)	119(3)
Mean	90(2)	Mean	118(2)
O(1)–Cu–O(5)	95(1)	C(1)–C(2)–C(3)	124(3)
O(2′)–Cu–O(5)	96(1)	C(1)–C(2)–C(7)	116(3)
O(3)–Cu–O(5)	95(1)	C(8)–C(9)–C(10)	125(3)
O(4′)–Cu–O(5)	97(1)	C(8)–C(9)–C(14)	114(3)
Mean	96(1)	Br(1)–C(3)–C(2)	126(3)
O(1)–Cu–Cu′	82·4(7)	Br(1)–C(3)–C(4)	115(3)
O(2′)–Cu–Cu′	86·5(6)	Br(2)–C(10)–C(9)	126(2)
O(3)–Cu–Cu′	82·5(6)	Br(2)–C(10)–C(11)	114(2)
O(4′)–Cu–Cu′	85·7(7)	C(3)–C(2)–C(7)	120(3)
Mean	84(2)	C(2)–C(3)–C(4)	119(3)
O(5)–Cu–Cu′	176·5(7)	C(3)–C(4)–C(5)	121(3)
Cu–O(1)–C(1)	124(2)	C(4)–C(5)–C(6)	121(3)
Cu′–O(2)–C(1)	121(2)	C(5)–C(6)–C(7)	117(3)
Cu–O(3)–C(8)	126(2)	C(6)–C(7)–C(2)	122(3)
Cu′–O(4)–C(8)	123(2)	C(10)–C(9)–C(14)	121(3)
Mean	125(2)	C(9)–C(10)–C(11)	120(3)
		C(10)–C(11)–C(12)	122(3)
		C(11)–C(12)–C(13)	117(3)
		C(12)–C(13)–C(14)	122(3)
		C(13)–C(14)–C(9)	117(3)
		Mean	120(2)

TABLE 4

Selected nonbonded contacts $< 3·5$ Å

(*a*) Intramolecular

O(1) · · · O(2)	2·24(3)	O(5) · · · O(1)	3·08(3)
O(3) · · · O(4)	2·22(3)	O(5) · · · O(2′)	3·07(3)
Br(1) · · · O(2)	2·94(2)	O(5) · · · O(3)	3·07(3)
Br(2) · · · O(3)	2·98(2)	O(5) · · · O(4′)	3·12(3)
O(1) · · · O(3)	2·84(3)	Cu′ · · · O(1)	3·09(2)
O(1) · · · O(4′)	2·83(3)	Cu′ · · · O(2′)	3·08(2)
O(2′) · · · O(3)	2·76(3)	Cu′ · · · O(3)	3·18(2)
O(2′) · · · O(4′)	2·76(3)	Cu′ · · · O(4′)	3·18(2)

TABLE 4 (*Continued*)

(*b*) Intermolecular

* O(4) · · · O(5$^{\mathrm{I}}$)	2·89(3)	C(2) · · · C(12$^{\mathrm{III}}$)	3·38(5)
O(2) · · · O(5$^{\mathrm{I}}$)	3·18(3)	O(5) · · · C(6′$^{\mathrm{IV}}$)	3·44(4)
O(5) · · · O(5′$^{\mathrm{II}}$)	3·23(5)	O(5) · · · C(5′$^{\mathrm{IV}}$)	3·46(5)

O(4) · · · H–O(5)			
O · · · O	2·89(3)Å	Cu–O(4) · · · O(5)	95(1)°
Cu–O(5) · · · O(4)	134(1)°	C(8)–O(4) · · · O(5)	121(3)°

* Probable hydrogen bond.

Roman numerals as superscripts refer to the following equivalent positions relative to the reference molecule at x, y, z:

I $1 + x, y, z$	III $1 + x, 1 + y, 1 + z$
II $x - 1, y, z$	IV $x, y, 1 + z$

TABLE 5

Equations of some weighted ($w = 1/\sigma^2$) least-squares planes in the form $lX + mY + nZ + p = 0$ where X, Y, and Z are orthogonal co-ordinates in Å referred to the crystallographic axes a, b, c^*. Deviations (Å) of relevant atoms from the planes are given in square brackets

	l	m	n	p
Plane (1):				
C(1)—(7), Br(1)	−0·3550	0·8996	−0·2545	0·2339

[C(1) 0·0432, C(2) −0·0555, C(3) 0·0344, C(4) 0·0299, C(5) −0·0072, C(6) 0·0066, C(7) −0·0092, Br(1) −0·0003]

	l	m	n	p
Plane (2):				
C(8)—(14), Br(2)	−0·4673	−0·5705	−0·6754	−0·5652

[C(8) −0·0525, C(9) 0·0194, C(10) 0·0407, C(11) −0·0479, C(12) −0·0335, C(13) −0·0173, C(14) 0·0643, Br(2) 0·0003]

	l	m	n	p
Plane (3):				
O(1), O(2), C(1), C(2)	−0·3000	0·9311	−0·2076	0·0195

[O(1) 0·0002, O(2) 0·0002, C(1) −0·0013, C(2) 0·0003]

	l	m	n	p
Plane (4):				
O(3), O(4), C(8), C(9)	−0·1456	−0·4785	−0·8659	−0·4689

[O(3) 0·0003, O(4), 0·0003, C(8) −0·0012, C(9) 0·0004]

	l	m	n	p
Plane (5):				
O(1), O(2′), O(3), O(4′)	0·8973	0·2576	−0·3585	1·1115

[O(1) −0·0071, O(2′) 0·0067, O(3) −0·0063, O(4′) 0·0070, Cu −0·1993]

	l	m	n	p
Plane (6):				
Cu, O(1), O(2), O(5)	−0·3161	0·9296	−0·1896	0

[Cu 0·0048, O(1) 0·0271, O(2) −0·0201, O(5) −0·0810, Cu′ − 0·0048, O(1′) −0·0271, O(2′) 0·0201, O(5′) 0·0810]

	l	m	n	p
Plane (7):				
Cu, O(3)—(5)	−0·2542	−0·2749	−0·9273	0

[Cu 0·0041, O(3) 0·0391, O(4) −0·0364, O(5) −0·0810, Cu′ −0·0041, O(3′) −0·0391, O(4′) 0·0364, O(5′) 0·0810]

Angles (°) between the planes:

(1)–(2)	100	(3)–(4)	103
(1)–(3)	5	(3)–(5)	87
(1)–(4)	100	(3)–(6)	1
(1)–(5)	90	(3)–(7)	89
(1)–(6)	5	(4)–(5)	87
(1)–(7)	85	(4)–(6)	104
(2)–(3)	105	(4)–(7)	14
(2)–(4)	22	(5)–(6)	89
(2)–(5)	109	(5)–(7)	89
(2)–(6)	105	(6)–(7)	90
(2)–(7)	26		

standard deviations, are given in Tables 2 and 3, non-bonded in Table 4, and some weighted least-squares mean planes in Table 5.

The crystal structure consists of centrosymmetric dinuclear units (Figure 1), with four bidentate *o*-bromobenzoate anions forming *syn–syn* bridges between the two copper atoms which are separated by 2·624(7) Å. The co-ordination about the copper atoms is octahedral. Five of its nearest neighbours are oxygen atoms, four of these being from the carboxylate anions, and the fifth from the water molecule. The four carboxylate oxygens are coplanar at distances from 1·96 to 2·01 Å (mean 1·99 Å) from the copper atom. The Cu–O(5) bond (2·17 Å) is nearly perpendicular to the plane of the carboxylate oxygen atoms so that the oxygen atoms form a tetragonal pyramid about the copper atom. The tetragonally distorted octahedron is completed by the centrosymmetrically related copper atom Cu′. Figure 2 shows the co-ordination polyhedron of the copper atom, which is displaced 0·20 Å in the direction of O(5) from the plane of the carboxylate oxygens (Table 5). This results in a nearly regular tetragonal distortion of the octahedron: the Cu′ · · · O(carboxylate) distances [3·08—3·18, mean 3·13 Å] are almost the same as the O(5) · · · O(carboxylate) distances [3·07—3·12, mean 3·09 Å] and the O · · · O distances are 2·76—2·84, mean 2·80 Å.

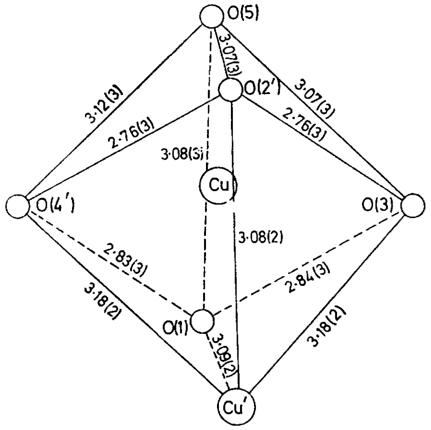

FIGURE 2 Co-ordination polyhedron of the copper atom

The central region of the molecule consists of two planes [planes (6) and (7) in Table 5], which are at right angles, O(5) being slightly displaced, by 0·08 Å, from each plane. One *o*-bromophenyl group, Br(1), C(2)—(7), is nearly coplanar with its carboxy-group (dihedral angle 5°), while the second group, Br(2), C(9)—(14), makes an angle of 22° with its carboxy-group. The *o*-bromobenzoate groups have similar bond lengths and angles.

The bond distances and angles involving the copper atoms, carboxylate groups, and O(5) are similar to those reported for a number of other dinuclear copper(II) carboxylate monoadducts (Table 6). The Cu–Cu distance of 2·624(7) Å agrees well with the 2·621(8) Å found for the aspirinate derivative,[13] the only other arylcarboxylate complex for which structural data are available. The Cu′–Cu–O(5) grouping is slightly non-linear [176·5(7)°], as in some of the other structures.[12,16] The mean bridging path-length (Cu–O–C–O–Cu′) is 6·50(3) Å, which is slightly, but not significantly, longer than the mean value [6·45(5) Å] for all the compounds listed in Table 6. This parameter remains constant despite differences in the Cu–O and C–O distances between the individual compounds.

TABLE 6

Comparison of structural parameters for compounds $Cu_2(RCO_2)_4L_2$

RCO_2^-	*o*-$BrC_6H_4COO^-$	HCO_2^-			$CH_3CO_2^-$					Succinate	Aspirinate
L	H_2O	NCS [a]	Urea [b]	½Dioxan [c]	H_2O [d]	NCS [a]	py(monoclinic) [e]	py(orthorhombic) [f]	Quinoline [g]	H_2O [h]	Acetyl oxygen [i]
(*a*) Mean bond distances (Å)											
Cu–Cu	2·624(7)	2·716(2)	2·657(7)	2·58(1)	2·614	2·643(3)	2·630(3)	2·645(3)	2·642	2·610(1)	2·621(8)
Cu–O	1·99(3)	1·983(4)	1·95(1)	1·96	1·967	2·03(1)	1·98(1)	1·96(2)	1·93	1·975(3)	1·96
Cu–O or Cu–N*	2·17(2)	2·09(1)*	2·11(1)	2·26	2·162	2·08(1)*	2·126(4)*	2·186(8)*	2·17*	2·102(7)	2·24(3)
C–O	1·26(2)	1·244(8)	1·27(3)	1·24	1·259	1·24(2)	1·24(2)	1·25(2)	1·24	1·262(5)	
(*b*) Mean bond angles (°)											
O–Cu–O (*cis* in planar group)	90(1)		89(1)				88·6(6)	89·3	89·4	89·5(3)	
O–Cu–O (*trans* in planar group)	168·5(5)		167·3(2)						167·8	168·5(3)	
O–Cu–O or O–Cu–N	96(1)		96							96	
Cu–Cu–O(carboxylate)	84(2)	83·0(1)	83·6(25)	85		84·0(3)		84		84	
Cu–Cu–O or Cu–Cu–N*	176·5(7)		174·0(4)	175							
Cu–O–C(carboxylate)	125(2)	122·7(3)	125			123(1)	124			124	
O–C–O(carboxylate)	124(3)	128·4(5)	122(2)	129		126(1)	125	125·6	130	124	
O–C–C(carboxylate)	118(2)			109			116(2)	118·6	115	118	
(*c*) Mean bridging path-length (Å)											
	6·50(3)	6·45	6·45	6·40	6·45	6·54	6·44	6·42	6·34	6·47	

[a] Ref. 15. [b] Ref. 16. [c] Ref. 12. [d] Refs. 7 and 8. [e] Ref. 9. [f] Ref. 10. [g] Ref. 14. [h] Ref. 11. [i] Ref. 13.

None of the four C–O(carboxylate) distances is significantly different from the mean value of 1·26 Å, which agrees with the accepted value.[27] The C–Br (mean 1·89), C–C(aromatic) (mean 1·41), and C(ar)–CO (mean 1·525 Å), distances are all close to normal.[27]

The bond angles about all the atoms are normal except those involving C(2), C(3), C(9), and C(10). Close contacts between Br(1) and O(2) [2·94(2)] and Br(2) and O(3) [2·98(2) Å], are responsible for expansion of the angles C(1)–C(2)–C(3) 124(3), Br(1)–C(3)–C(2) 126(3), C(8)–C(9)–C(10) 125(3), and Br(2)–C(10)–C(9)

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[27] *Chem. Soc. Special Publ.*, No. 11, 1958, and No. 18, 1965.

126(2)°, and corresponding contractions of the angles C(1)–C(2)–C(7) 115(3), Br(1)–C(3)–C(4) 115(3), C(9)–C(10)–C(14) 114(3), and Br(2)–C(10)–C(11) 114(2)°, from the expected 120°.

The crystal packing arrangements, viewed down *a* and *c*, are shown in Figures 3 and 4 respectively. Probable hydrogen bonds, O(4) ··· O(5^{I}) [O ··· O 2·89(3) Å], shown as broken lines in Figure 4, join the dinuclear units into infinite chains along *a*. The geometrical data for the hydrogen bonding scheme (see Table 4) are normal. All other intermolecular contacts correspond to van der Waals interactions; those <3·5 Å are listed in Table 4.

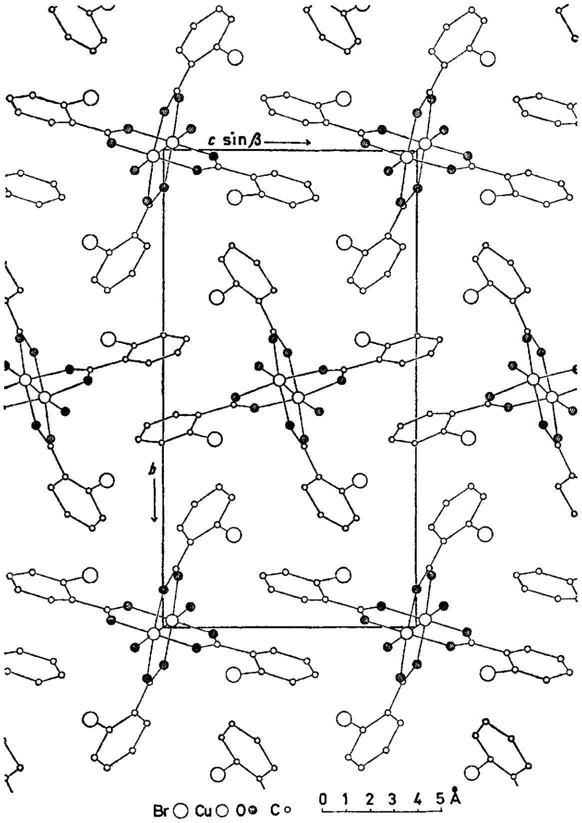

Figure 3 Projection of the structure down *a*

At this point there is no simple correlation between the structural parameters, in particular the Cu–Cu, Cu–O, and Cu–O–C–O–Cu′ distances, and the magnetic properties of the copper(II) carboxylates. The magnitude of the magnetic exchange interaction is highly dependent on the identity of the parent acid and the adduct, in cases where one is present.

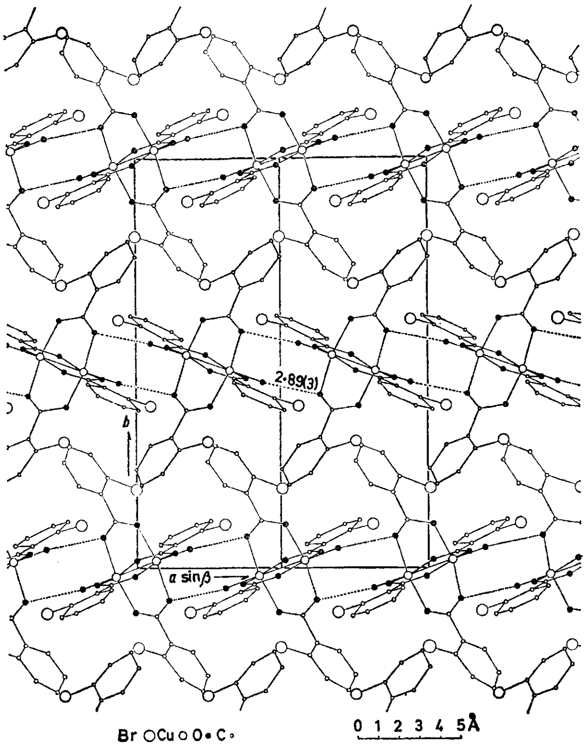

Figure 4 Projection of the structure down *c*; the broken lines indicate probable hydrogen bonds

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