Anhydrous Copper(II) Decanoate

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Abstract. $Cu[CH_3(CH_2)_8COO]_2$, triclinic, $P\bar{1}$, $a = 7\cdot94$ (1), $b = 5\cdot28$ (3), $c = 28\cdot13$ (5) Å; $\alpha = 94\cdot6$ (10), $\beta = 97\cdot1$ (5), $\gamma = 98\cdot6$ (10)°; $Z = 2$, $M = 406$; $D_c = 1\cdot170$ (6), $D_m = 1\cdot17$ (2) g cm^{-3}. Each copper atom is approximately octahedrally coordinated, its neighbours being one copper atom, four oxygen atoms from the same cell and one oxygen atom from a neighbouring cell. The hydrocarbon chains are packed in accordance with a common triclinic subcell.

Introduction. The crystals used in this investigation were obtained by a gel diffusion method as described by Bridle & Lomer (1965). Aqueous solutions of potassium decanoate and copper sulphate were allowed to diffuse into a column of silica gel from opposite ends and after several months clusters of needle-shaped crystals formed in the gel. These were removed from the gel and cleaned by repeated washing with ethanol. The crystals obtained were bright blue-green in colour and were extremely fragile and easily deformed during manipulation. Many apparently single crystals as viewed in a polarizing microscope turned out to be bundles of smaller crystals stuck together with a common axis, subsequently called the b axis. Ultimately one crystal, though not of good quality, was selected and zero, first and second-layer photographs were taken for full 360° rotation of the crystal about its b axis, using filtered Cu $K\alpha$ radiation. Partly because of the poor quality of the crystal and partly because of the relatively long c edge of the unit-cell it was not possible to take integrated photographs, and the intensities had to be visually estimated by comparison with an intensity scale. Because of the fragile and needle-shaped character of the crystals it was not feasible to record data with the crystal rotating about a second axis. 363 independent non-zero reflexions were measured out of a possible 1250 reflexions observable with copper radiation. No reflexions with $(\sin \theta)/\lambda > 0\cdot5$ Å^{-1} were observed. Because of the small dimensions of the crystal in planes nearly perpendicular to the b axis, ($\simeq 0\cdot05$ mm) and the small absorption coefficient ($\mu = 1\cdot46$ mm^{-1}) no absorption corrections were applied.

A trial structure in which the copper atom environment was the same as that found in copper butyrate by Bird & Lomer (1972), and in which the hydrocarbon chain directions were determined by inspection of Pat-

terson syntheses was used and successfully refined by standard least-squares methods. Hydrogen atoms were placed in calculated positions in the final stages of the calculations but their parameters were not refined. Individual isotropic temperature factors were refined for all the heavy atoms; the final R value was $0\cdot134$. The atomic coordinates and temperature factors are given in Table 1.†

Table 1. *Atom parameters: coordinates as fractions of the unit-cell edges* ($\times 10^3$) *and temperature factors in* Å^2

The standard deviations given in parentheses are in units corresponding to the least significant digit in the parameters.

	x/a	y/b	z/c	B
C(1)	198 (5)	63 (9)	81 (2)	1·4 (10)
C(2)	311 (7)	78 (11)	129 (2)	6·0 (17)
C(3)	291 (6)	307 (9)	163 (2)	3·5 (13)
C(4)	402 (6)	297 (9)	215 (2)	4·1 (14)
C(5)	398 (7)	542 (10)	250 (2)	5·0 (15)
C(6)	517 (6)	532 (9)	298 (2)	3·9 (14)
C(7)	503 (5)	761 (8)	335 (2)	2·4 (12)
C(8)	621 (6)	752 (10)	385 (2)	4·3 (14)
C(9)	626 (7)	999 (9)	419 (2)	5·9 (16)
C(10)	726 (9)	990 (9)	467 (2)	10·4 (22)
C(11)	788 (6)	735 (9)	44 (2)	1·8 (17)
C(12)	657 (6)	557 (9)	73 (2)	2·4 (12)
C(13)	745 (6)	527 (9)	124 (2)	4·1 (15)
C(14)	780 (6)	807 (9)	154 (2)	3·6 (14)
C(15)	886 (7)	781 (9)	202 (2)	4·6 (15)
C(16)	898 (7)	30 (10)	241 (2)	5·4 (16)
C(17)	3 (6)	5 (9)	291 (2)	3·8 (14)
C(18)	998 (7)	247 (10)	328 (2)	6·2 (17)
C(19)	114 (8)	207 (12)	380 (2)	7·2 (18)
C(20)	111 (10)	453 (12)	418 (3)	11·1 (25)
O(1)	93 (4)	202 (6)	69 (1)	3·6 (9)
O(2)	215 (4)	876 (6)	55 (1)	3·3 (9)
O(3)	752 (6)	96 (6)	36 (2)	3·3 (9)
O(4)	875 (6)	604 (8)	22 (1)	2·3 (9)
Cu	930 (1)	200 (1)	13 (1)	2·9 (2)

Discussion. Diagrams of the structure projected on to planes perpendicular to the a and b axes are shown in Fig. 1. The structure contains centrosymmetric dimers with coordination of the copper and oxygen atoms, shown in Fig. 2, similar to that in copper butyrate (Bird & Lomer, 1972) and to that in copper acetate monohydrate (Van Niekerk & Schoening, 1953).

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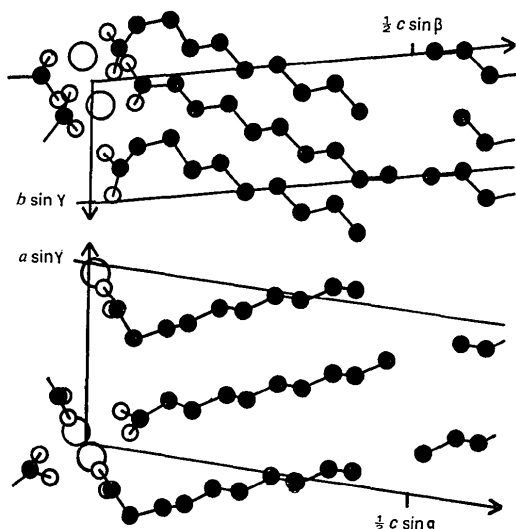
Fig. 1. Projections of the structure of copper decanoate along the a and b axes. Large circles are copper atoms, small open circles are oxygen atoms and small closed circles are carbon atoms.
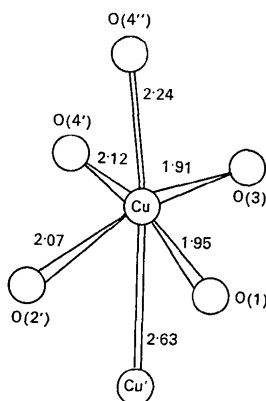

Fig. 2. Coordination of copper atoms in copper decanoate. The bond lengths are given in Å and have standard deviations of approximately 0·05 Å.

One of the pairs of hydrocarbon chains in each dimer has the carbon and oxygen atoms arranged in the common plane zigzag conformation throughout its length but the chains in the other pair are distorted near the carboxyl group by rotations about the bonds C(11)–C(12) and C(12)–C(13). The remainder of the atoms in these 'bent' chains, however, are arranged in the usual plane zigzag conformation, and pack together with those of the straight chains to form a structure which may be described by a triclinic subcell with dimensions $a=4\cdot42$, $b=5\cdot28$, $c=2\cdot56$ Å; $\alpha=70\cdot2$, $\beta=109\cdot6$, $\gamma=117\cdot5°$. These subcell dimensions are close to those reported in several other hydrocarbon chain compounds (see e.g. Lomer, 1963) and it is interesting that this close packing of the chains over part of their length is realized despite the distortion of some of them which is apparently necessary for the copper and oxygen atoms to achieve their favoured arrangement.

None of the C–C bond lengths or C–C–C bond angles differed significantly from the commonly accepted values, the mean observed values being $1\cdot57\pm0\cdot02$ and $110\cdot2\pm0\cdot5°$. The temperature factors of the carbon atoms in the methyl groups are very large. Similarly high temperature factors for atoms near the methyl group ends of hydrocarbon chains were observed in copper butyrate and also by Lewis & Lomer (1969) in potassium decanoate. It is not clear whether these high values are due to large thermal motions or to a degree of static disorder among the chains.

References

Bird, M. J. & Lomer, T. R. (1972). Acta Cryst. B28, 242–246.

Bridle, C. & Lomer, T. R. (1965). Acta Cryst. 19, 483.

Lewis, E. V. L. & Lomer, T. R. (1969). Acta Cryst. B25, 702–710.

Lomer, T. R. (1963). Acta Cryst. 16, 984–988.

Van Niekerk, J. N. & Schoening, F. R. L. (1953). Acta Cryst. 6, 227–232.

Anhydrous Copper(II) Octanoate

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Abstract. $Cu[CH_3(CH_2)_6COO]_2$, triclinic, $P\bar{1}$, $a=8\cdot80$ (2), $b=5\cdot20$ (1), $c=22\cdot06$ (1) Å; $\alpha=95\cdot1$ (5), $\beta=92\cdot4$ (5), $\gamma=110\cdot5$ (5)°, $Z=2$, $M=350$; $D_c=1\cdot230$ (6), $D_m=1\cdot21$ (4) g cm^{-3}. The copper atom environment is the same as that in copper decanoate but the packing of the hydrocarbon chains differs in detail.

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Introduction. Copper(II) octanoate was prepared by adding copper carbonate to an excess of solution of oc-