



Fig. 1. The crystal structure of cholesteryl laurate in projection down the b axis. Molecules A are close to the screw axis at $(\frac{1}{2}, y, 0)$. Molecules B are close to the screw axis at $(0, y, 0)$.

cules. There is almost no laurate-laurate packing. Most importantly, the packing of the laurate A and B chains with the cholesteryl groups might be relevant to the structural arrangement when cholesterol is incorporated in phospholipid bilayers (Huang, 1977).

Bond lengths and angles for cholesteryl laurate molecules A and B are consistent with those found in cholesteryl acetate (Sawzik & Craven, 1979), and in related crystal structures (Craven & Guerina, 1979b; Guerina & Craven, 1979; Craven & DeTitta, 1976). The apparent bond distances in the terminal region of the ester chains are shortened considerably as a result of large atomic thermal vibrations.

The tetracyclic ring systems of the two independent cholesteryl laurate molecules have similar conformations. A best least-squares fit for the superposition of the C(1)–C(19) fragment from A and B molecules (Nyburg, 1974) gave an average r.m.s. displacement for corresponding atoms of 0.091 Å. Differences in the conformation at the ester linkage follow the same pattern as in the nonanoate structure (Guerina & Craven, 1979). The C(2)–C(3)–O(3)–C(28) angle is 79° in cholesteryl laurate A and 127° for B . In both laurate molecules, the ester chains are almost fully extended, with torsion angles in the bonds along the chain from

C(29)–C(30) through C(37)–C(38) of $-170, 174, -179, 174, -167, 177, 171, 171, 167^\circ$ for molecule A and $-171, -170, -177, 175, -179, 159, -161, 179, -171^\circ$ for molecule B .

This work was supported by a grant (HL-20350) from the US Public Health Service, National Institutes of Health. Many of the computer programs used were written or modified by Dr R. Shiono.

References

- ABRAHAMSSON, S. & SELIN, K. (1963). *Acta Cryst.* **16**, A58.
 BARNARD, J. A. W. & LYDON, J. E. (1974). *Mol. Cryst. Liq. Cryst.* **26**, 285–296.
 BARRALL, E. M. II & JOHNSON, J. F. (1974). *Liquid Crystals and Plastic Crystals*, Vol. 2, edited by G. W. GRAY & P. A. WINDSOR, Ch. 10, pp. 814–822. New York: Wiley-Interscience.
 CRAVEN, B. M. & DETITTA, G. T. (1976). *J. Chem. Soc. Perkin Trans. 2*, pp. 814–822.
 CRAVEN, B. M. & GUERINA, N. G. (1979a). *Chem. Phys. Lipids*. In the press.
 CRAVEN, B. M. & GUERINA, N. G. (1979b). *Chem. Phys. Lipids*. Submitted.
 CROMER, D. T. & WABER, J. T. (1965). *Acta Cryst.* **18**, 104–109.
 DAHLÉN, B. (1979). *Chem. Phys. Lipids*. Submitted. [*Acta Cryst.* (1978). A **34**, S70. Abstr. No. 04.4-2.]
 DAVIS, G. J. & PORTER, R. S. (1970). *Mol. Cryst. Liq. Cryst.* **6**, 377–391.
 DAVIS, G. J., PORTER, R. S. & BARRALL, E. M. II (1970). *Mol. Cryst. Liq. Cryst.* **11**, 319–330.
 GUERINA, N. G. & CRAVEN, B. M. (1979). *J. Chem. Soc. Perkin Trans. 2*. In the press.
 HUANG, C. H. (1977). *Lipids*, **12**, 348–356.
 NYBURG, S. C. (1974). *Acta Cryst.* **B30**, 251–253.
 PATTABHI, V. & CRAVEN, B. M. (1979). *J. Lipid Res.* Submitted.
 SAWZIK, P. & CRAVEN, B. M. (1979). *Acta Cryst.* **B35**. In the press.
 STEWART, R. F., DAVIDSON, E. R. & SIMPSON, W. T. (1965). *J. Chem. Phys.* **42**, 3175–3187.

Acta Cryst. (1979). **B35**, 791

The crystal and molecular structures of magnesium di-*o*-phthalatocuprate(II) tetrahydrate and strontium di-*o*-phthalatocuprate(II) trihydrate: errata. By MARINA BIAGINI CINGI, ANNA MARIA MANOTTI LANFREDI, ANTONIO TIRIPICCHIO and MARISA TIRIPICCHIO CAMELLINI, *Istituto di Chimica Generale, Università di Parma, Centro di Studio per la Strutturistica Diffrattometrica del CNR, Parma, Italy*

(Received 6 November 1978; accepted 14 November 1978)

Abstract

The Mg compound, a tetrahydrate, was given by mistake as a dihydrate in the paper by Biagini Cingi, Manotti Lanfredi, Tiripicchio & Tiripicchio Camellini [*Acta Cryst.* (1978). **B34**, 406–411]. Thus the title, the formula and crystal data must be corrected to: title: The crystal and molecular

structure of magnesium di-*o*-phthalatocuprate(II) tetrahydrate; formula: $\text{Mg}[\text{Cu}(\text{C}_8\text{H}_4\text{O}_4)_2] \cdot 4\text{H}_2\text{O}$; crystal data: $\text{C}_{16}\text{H}_{16}\text{CuMgO}_{12}$, $M_r = 488.15$, $D_c = 1.76 \text{ Mg m}^{-3}$, $\mu(\text{Mo K}\alpha) = 1.283 \text{ mm}^{-1}$.

All information is given in the *Abstract*.

0567-7408/79/030791-01\$01.00

© 1979 International Union of Crystallography