

Acta Cryst. (1966). **20**, 309

Crystal data for (-)-threo-12,13-dihydroxyoleic acid. By DAVID A. LUTZ and WILLIAM E. SCOTT, *Eastern Utilization Research and Development Division, Agricultural Research Service, U.S. Department of Agriculture, Philadelphia, Pa. 19118, U.S.A.*

(Received 20 August 1965)

The present study was undertaken to obtain crystal data on (-)-threo-12,13-dihydroxyoleic acid, $C_{18}H_{34}O_4$, which was prepared by acetolysis of the seed oil of *Vernonia anthelmintica* (L.) Willd. (Scott, Krewson & Riemenschneider, 1962). The compound was further purified [as evidenced by chemical analysis (C 68.5, H 10.8%) and melting point (63–63.5°C)] and single crystals were produced by a series of slow crystallizations from acetone at room temperature. Cell constants were determined from various oscillation and Weissenberg photographs, using $Cu K\alpha$ radiation ($\lambda = 1.5418 \text{ \AA}$). The density was measured by flotation. The space group was determined from systematic extinctions ($h00$, $0k0$ and $00l$ absent for h , k or l odd). The crystal data are

as follows: $a = 5.05 \pm 0.01$, $b = 8.51 \pm 0.02$, $c = 44.66 \pm 0.05 \text{ \AA}$, $U = 1920 \text{ \AA}^3$, $z = 4$, $D_x = 1.088 \text{ g.cm}^{-3}$, $D_m = 1.085 \text{ g.cm}^{-3}$; space group, $P2_12_12_1$.

No further work on this compound is contemplated at present.

The authors would like to thank Dr Thomas H. Doyne of Villanova University for his assistance.

References

- SCOTT, W. E., KREWSON, C. F. & RIEMENSCHNEIDER, R. W. (1962), *Chem. and Ind.*, 2038.