

Acta Cryst. (1963). **16**, 434

Crystallographic data for methyl derivatives of benzoic acid. By J. L. ELIAS and S. GARCÍA-BLANCO, *Instituto de Física "Alonso de Santa Cruz", Madrid, Spain*

(Received 19 November 1962)

2,3,4-Trimethylbenzoic acid crystallizes from ethanol in the form of transparent crystals of tabular shape.

From goniometer measurements, rotating-crystal and Weissenberg photographs with Cu $K\alpha$ radiation, the following results were obtained:

Triclinic symmetry

$$a = 8.72, b = 7.55, c = 15.43 \text{ \AA}; \\ \alpha = 103^\circ 17', \beta = 107^\circ 10', \gamma = 93^\circ 6'.$$

The observed density obtained by the flotation method in aqueous solutions of sodium thiosulphate was 1.27 g.cm^{-3} , which agrees closely with a calculated density of 1.268 g.cm^{-3} for a unit cell containing four molecules. No further work on this compound is in progress.

***m*-Toluic acid** crystallizes from ethanol in the form of flat plates.

From goniometer measurements, rotating-crystal and Weissenberg photographs with Cu $K\alpha$ radiation, the following results were obtained:

Monoclinic symmetry

$$a = 10.53, b = 8.36, c = 16.54 \text{ \AA}, \beta = 92^\circ 30'.$$

Acta Cryst. (1963). **16**, 434

The unit cell and space group of voachalotine. By J. IBALL and C. H. MORGAN, *Chemistry Department, Queen's College, Dundee, Scotland*

(Received 5 November 1962)

Voachalotine is an indole alkaloid isolated from the bark of a Congolese tree, *Voacanga chalotiana* Pierre ex Stapf (Pecher, Defay, Gauthier, Peeters, Martin & Vandermeers, 1960). Colourless needles were obtained by recrystallization from a methanol-water mixture. These were monoclinic with unit cell dimensions

$$a = 20.79, b = 7.85, c = 23.65 \text{ \AA}, \beta = 91^\circ 57'.$$

The density was determined by flotation in a density gradient column which was accurately calibrated. The observed value 1.256 g.cm^{-3} agrees well with the value (1.261) calculated from the unit-cell dimensions, if it is assumed that there are 8 molecules of $\text{C}_{22}\text{H}_{26}\text{O}_3\text{N}_2$ per unit cell. The original purpose of the investigation was to obtain a value for the molecular weight; the experimental value is 365, which compares with 366 determined by mass spectrometer (Pecher *et al.*, 1961) and with a theoretical value of 366.4.

The systematic absences observed on Weissenberg photographs were hkl absent if $h+k$ is odd. There are three space groups which are possible according to this

The observed density of 1.26 g.cm^{-3} fits well with eight molecules per unit cell and the calculated density is 1.234 g.cm^{-3} .

The observed systematic absences correspond to the space group $P2_1/c(C_{2h}^5)$ in accordance with the data published by Srivastava (1959).

No further work on this compound is in progress.

2,6-Dimethylbenzoic acid crystallizes from ethanol-chloroform solution in tabular crystals.

From goniometer measurements, rotating-crystal and Weissenberg photographs with Cu $K\alpha$ radiation, the following results were obtained:

Monoclinic symmetry

$$a = 15.24, b = 4.04, c = 13.16 \text{ \AA}, \beta = 94^\circ 8'.$$

The density experimentally determined by the flotation method is 1.20 g.cm^{-3} . There are four molecules per unit cell and the calculated density is 1.227 g.cm^{-3} .

The observed systematic absences $h0l$ with $l = 2n + 1$, $0k0$ with $k = 2n + 1$ correspond to the space group $P2_1/a(C_{2h}^2)$.

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observation, $C2$, Cm and $C2/m$, but since the compound is optically active the space group must be $C2$ and there are two molecules per asymmetric unit.

It has now been shown (Defay, Kaisin, Pecher & Martin, 1961) that voachalotine has a structure which is very similar to that of macusine A (McPhail, Robertson, Sim, Battersby, Hodson & Yeowell, 1961).

We are indebted to Prof. R. H. Martin (Brussels) for supplying the crystals and to the British Empire Cancer Campaign for financial support.

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