

AN X-RAY INVESTIGATION OF A CRYSTAL OF METHYL MERISTOTROPATE

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It has been reported previously that the suggested structure for meristotropic acid is 3-hydroxy-6-11(12),13(18)-dien-29-oic acid. The position of the keto group was determined on the basis of NMR spectra [1].

In the present work we have obtained preliminary x-ray characteristics of the methyl ester of meristotropic acid (MA), $C_{31}H_{46}O_4$.

The methyl ester was isolated by recrystallizing MA from ethanol and prolonged standing. The crystals had mp 280–281°C. The habitus of the crystals was elongated and prismatic, with the frequent occurrence of twinned specimens.

Single crystals were studied by Laue x-radiographic method of oscillating and reciprocal-lattice diagrams. The following parameters were obtained for the primitive rhombic cell: $a=12.1 \text{ \AA}$, $b=27.1 \text{ \AA}$, $c=7.35 \text{ \AA}$.

On the reciprocal-lattice diagrams, the layer lines around C of reflections of the $h00$ and $0k0$ types are also present in which $h=2n$ and $k=2n$. No systematic extinctions were observed for hkL . On the $0kl$ reciprocal-lattice diagrams, reflections of the $0k0$ type obey the condition $k=2n$, while for reflections of the $00l$ and also of the Hkl types there are no limitations.

Thus, an analysis of the systematic extinctions indicated leads to the space group $D_2^3 = P 2,2,2$.

At a density of $\rho=1.18$ of the crystals of the methyl ester of MA, there are four formula units, $C_{31}H_{46}O_4$, packed into the rhombic cell.

LITERATURE CITED

1. N. P. Kir'yalov and G. S. Amirova, *Khim. Prirodn. Soedin.*, 60 (1968).

Institute of Inorganic and Physical Chemistry, Academy of Sciences of the Azerbaidzhan SSR. Institute of Botany, Academy of Sciences of the Azerbaidzhan SSR. Translated from *Khimiya Prirodnikh Soedinenii*, No. 5, pp. 661–662, September–October, 1972. Original article submitted February 22, 1972.

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