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AN X-RAY DIFFRACTION INVESTIGATION OF A SINGLE CRYSTAL OF METHYL TRIPHYLLATE

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Methyl triphyllate (MT) has been isolated from the neutral products of the hydrolysis of an extract of the roots of *Glycyrrhiza triphylla* Fisch. et Mey [1]. Its composition has been established as $C_{31}H_{48}O_5$, mp 268–270°C. A single crystal of MT was obtained by recrystallization from ethanolic solution.

We have previously [2] reported x-ray structural investigations of another natural tri-terpene — methyl meristotropate. In the present paper we give preliminary x-ray diffraction results on MT. The parameters of the elementary cell were determined from rocking x-ray diffraction patterns and Weissenberg patterns with copper radiation.

The parameters were defined by the method of least squares for 12 reflections on a Hilger-Watts automatic four-circle x-ray diffractometer:

$$\begin{aligned}a &= 12.766(1) \text{ \AA}, \\b &= 31.882(1) \text{ \AA}, \\c &= 6.858(1) \text{ \AA}, \\\gamma &= 90.53(1)^\circ.\end{aligned}$$

Monoclinic System. Taking systematic extinctions into account leads to the space groups B2 and B2/m. The number of molecules per elementary cell found on the basis of the molecular weight and the density ($Z = 4$) unambiguously determines the space group B2.

A three-dimensional set of intensities consisting of 1804 independent reflections ($\lambda_{Cu\alpha} = 1.5418 \text{ \AA}$) has been obtained on the diffractometer mentioned.

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