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Short Communications

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Structure of morellin. By B. DAYAL and S. C. MATHUR, *Department of Physics, Banaras Hindu University, India*

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Morellin is an antibiotic, extracted from the seeds of an Indian tropical evergreen *Carcinia Morella* (Mysore Gamboge tree); the yellow tetragonal crystals show positive birefringence, with marked elongation along [001] and a tendency to cleave very easily parallel to (110). The unit-cell dimensions, $a=15.7$, $c=11.7$ Å, are in good agreement with those given by Kartha (1954a). The empirical formula $C_{33}H_{38}O_7$ gives four molecules in the unit cell and the space group is $P4_1$ (Kartha, 1954b).

The provisional chemical formula suggested by Venkataraman in a private communication includes a chromene nucleus and an attached side-chain. The very marked yellow colour of the crystals suggests the presence of a chromophore such as a highly conjugated polycyclic system; the X-ray investigation briefly referred to in this communication confirms this view.

So far only Weissenberg photographs have been taken for $hk0$ and $0kl$ reflections and the intensities have been visually estimated. A very strong 430 reflection, together with the observed cleavage along (110) indicates that the flat ring system is lying nearly parallel to this plane with the longer axis of the molecule lying approximately parallel to the tetrad axis of the crystal. From packing considerations it was possible to give a sign to the 430 reflection and to a few others. An electron-density map calculated on this projection (Fig. 2) is consistent with the presence of a ring-system seen end-on and an additional group attached to the molecule.

A Patterson projection on (010) showed a strong maximum on the c axis at about 4 Å from the origin. This and other vector features were again consistent with a polycyclic ring system in spite of the overlapping molecules seen on this projected view of the crystal.

Trials of atomic positions based on the formula of

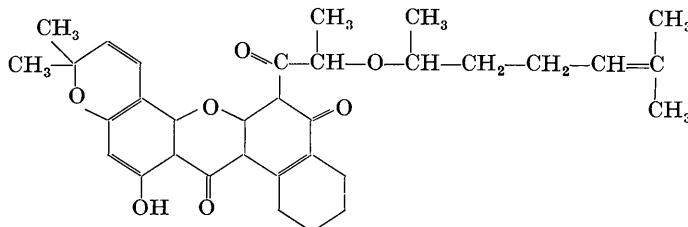


Fig. 1. Provisional chemical formula of morellin.

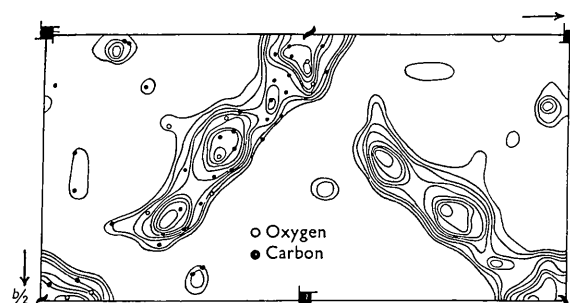


Fig. 2. Fourier projection of morellin on the (001) plane along with the atoms of the quarter unit cell projected on the same plane, only half of the unit cell has been drawn.

Fig. 1 have shown reasonable agreement between calculated and observed structure factors but, owing to the complexity of the molecule and its awkward projections on (001) and (010), are not sensitive to further refinement. It is clear that the analysis needs to be carried out in three dimensions and this is now being done.

The crystals for this investigation were kindly provided by Dr K. Venkataraman, Director of the National Chemical Laboratory, India. One of us (B. D.) would like to thank Prof. J. D. Bernal, F.R.S., of Birkbeck College, London, for hospitality in his laboratory where part of this work was carried out, and he is grateful to Dr C. H. Carlisle for help and encouragement.

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