

X-Ray Crystal Structure Revision for the Fungal Metabolite (\pm)-Altenuene

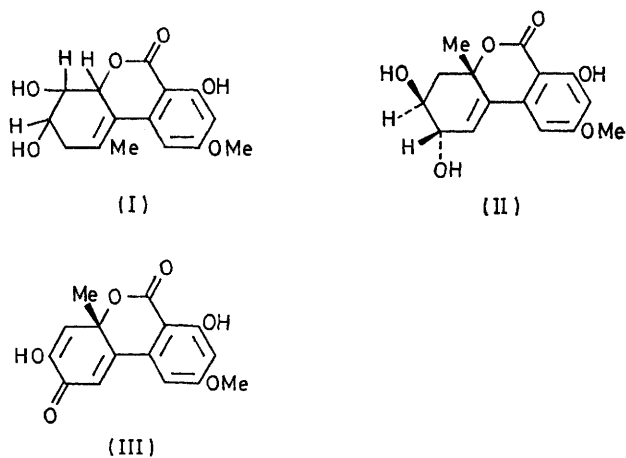
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Summary The structure of the fungal metabolite (\pm)-altenuene has been elucidated by direct method X-ray crystal structure analysis.



On the basis of extensive spectroscopic studies structure (I) with undefined stereochemistry was earlier assigned to (\pm)-altenuene,¹ C₁₅H₁₆O₆, a toxic fungal metabolite from *Alternaria tenuis*.^{2,3} We have conducted a single-crystal X-ray analysis which now establishes unequivocally that (\pm)-altenuene is correctly represented by formula (II) and its mirror image.

(\pm)-Altenuene crystallizes from acetone-hexane as colourless prisms, m.p. 190–191°, belonging to the triclinic system, space group $P\bar{1}$, with $a = 12.61(2)$, $b = 7.98(1)$, $c = 8.50(1)$ Å, $\alpha = 102.9(2)$, $\beta = 100.2(2)$, $\gamma = 116.5(2)^\circ$, $Z = 2$. The structure was solved using the programme MULTAN⁴ and employing 279 $|E|$ values ≥ 1.3 . Molecular parameters were refined by full-matrix calculations to a current R of 0.14 over 1715 independent reflexions from photographic data.

This revised structure for (\pm)-altenuene is similar to that

recently reported⁵ for (\pm)-dehydroaltenuis (III) which is a potential precursor in a biosynthetic sequence.

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⁴ G. Germain, P. Main, and M. M. Woolfson, *Acta Cryst.*, 1971, **A27**, 368.

⁵ D. Rogers, D. J. Williams, and R. Thomas, *Chem. Comm.*, 1971, 393.