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THE MOLECULAR STRUCTURE OF PHASEOLLIN

C. DeMartinis*, M.F. Mackay*, Dawn R. Perrin+ and B.J. Poppleton#

* Department of Physical Chemistry, La Trobe University, Bundoora, Victoria, Australia 3083.

+ Division of Plant Industry, C.S.I.R.O., P.O. Box 1600, Canberra, A.C.T., Australia 2601.

Division of Applied Organic Chemistry, C.S.I.R.O., Box 4331 G.P.O., Melbourne, Victoria Australia 3001 and Division of Chemical Physics, C.S.I.R.O., P.O. Box 160, Clayton, Victoria, Australia 3168.

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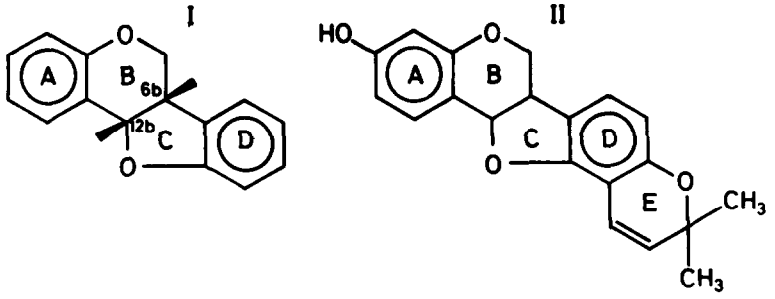
Phaseollin, $C_{20}H_{18}O_4$, a lipophilic antifungal compound isolated from *Phaseolus vulgaris L.* (1), is a member of a group of naturally occurring antifungal pterocarpans which have the basic ring structure (I) with asymmetric centres at C-6b and C-12b. A *cis* B/C ring junction has been reported (2). From ultraviolet (1), infrared and NMR (3) spectra the molecular skeleton (II) has been assigned to phaseollin. Results of some earlier studies of pterocarpans and related compounds led to a proposal that the characteristic antifungal activity of the compounds may depend on their molecular shape (4). An X-ray analysis of crystals of phaseollin consequently was undertaken to define the conformational detail in the molecule, and thus establish the conformation of the benzofurobenzopyran ring system.



Crystals of phaseollin, $C_{20}H_{18}O_4$, are orthorhombic and belong to the space group $P2_12_12_1$ with a = 6.540(3), b = 12.975(6), c = 19.388(4) Å and Z = 4. The structure was solved by direct methods using the *X-RAY* system (5), and refined with 992 terms ($F_o > 3\sigma F_o$) measured on a Rigaku-*AFC* four-circle diffractometer with CuKα radiation. Refinement of the non-hydrogen atoms with anisotropic temperature factors has yielded a reliability index, $R = \Sigma\Delta F_o/\Sigma F_o$ of 0.083. Calculated hydrogen atom coordinates were included in the final refinements but they

were not varied.

The molecular formula (II) is confirmed and a perspective view of the molecule is given in Fig.1. Phaseollin is approximately propeller in shape and apart from C(3) of ring E and the methyl carbon C(3B), the non-hydrogen atoms lie nearly in two planes which are mutually inclined at *ca.* 51°. The B/C ring junction is *cis*. The staggered conformation of the benzofurobenzopyran ring system, with the torsion angle O(8)[C(7),C(6B)]C(12B) = 56.3°, agrees with the assignment based on proton magnetic resonance data (6). Ring C is envelope with C(12B) lying +0.44 Å out-of-plane, while ring B is skewed, C(6B) and C(7) lying +0.12 and -0.55 Å respectively from the plane of the other ring atoms. By virtue of the double bond between C(1) and C(2) and its fusion to ring D, ring E is a distorted half-chair, C(2) and C(3) deviating from the coplanarity of the other four atoms by -0.32 and -0.69 Å respectively.

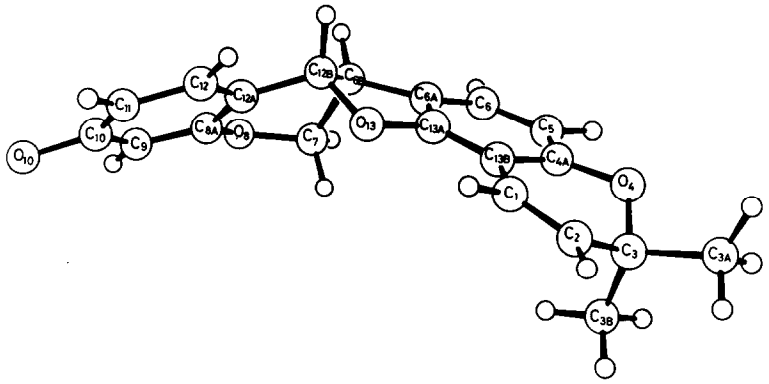


Fig. 1.

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