

## SHORT COMMUNICATIONS

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**The crystal structures and absolute stereochemistries of monobromoisodehydrobispulegone and dibromodehydrobispulegone.** By D. ROGERS, *Chemical Crystallography Laboratory, Imperial College, London, SW7 2AY, England* and J. M. FRANCO, S. MARTÍNEZ-CARRERA and S. GARCÍA-BLANCO, *Instituto de Química-Física 'Rocasolano', C.S.I.C., Serrano 119, Madrid 6, Spain*

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The compound whose structure was reported in *Acta Cryst.* (1974), B30, 415 was wrongly named. It was monobromoisodehydrobispulegone (m.p. 251 °C dec.;  $[\alpha]_D^{20} = +54.2^\circ$ ). With this revision and by comparison with the earlier report of the structure of dibromodehydrobispulegone it is possible to define unambiguously the distinction between the stereochemistries of the nor and iso series of bispulegone isomers, and to assign the absolute configurations of the two compounds.

Recent correspondence between the authors has drawn attention to an inconsistency between the names and the stereochemistries of two derivatives of bispulegone whose crystal structures have been reported, *viz.* dibromodehydrobispulegone (I) (Perales, Martínez-Carrera & García-Blanco, 1969) and monobromodehydrobispulegone (II) (Franco, Martínez-Carrera & García-Blanco, 1974). Reference to Professor J. Pascual, who supplied both specimens, reveals that (I), which is characterized by m.p. 188–9 °C,  $[\alpha]_D^{20} = -92.9^\circ$  and is a member of the so-called nor series of bispulegone isomers, is correctly named, but that (II) (m.p. 251 °C dec.,  $[\alpha]_D^{20} = +54.2^\circ$ ) is in the iso series and should, therefore, be called monobromoisodehydrobispulegone.

With this correction, the stereochemical distinction between the nor and iso carbon skeletons becomes consistent, *i.e.* they are epimeric at C(12) (our numbering) as shown below.

Unfortunately, this result is the opposite of that arbitrarily assumed by J. Pascual and co-workers (Bartual, Camps, Parés & Pascual, 1968; Bartual, Camps, Ferrer, Pascual & Roqué, 1970; Bartual & Pascual, 1970; Bartual, Font, Forné, Pascual & Roqué, 1972; Font-Cistero & Pascual, 1974). The above skeletons are achiral, but, though it was not discussed in the two above-mentioned X-ray papers, it is possible to assign the position of the carbonyl (at C(14) in each compound) and thus their absolute configurations from the knowledge that they were obtained by dimerization of (+)-pulegone which imparts an *R* configuration at atom C(12). Both were then brominated at C(13). They are respectively correctly depicted in Fig. 6 of the 1969 paper and Fig. 1 of the 1974 paper (though not all the other Figures are consistent, however), and both coordinate lists give molecules of the correct chirality when referred to right-handed axes.

The chemical implications of these and other results are discussed in two papers to be submitted to *J. Chem. Soc. Perkin* by Rogers, Quick & McConway, and by Forné & Pascual.

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