The Stereochemistry of Plathyterpol, a Diterpene with A:B-cis-Ring Fusion

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Summary The absolute stereochemistry of plathyterpol at all centres except C-13 is defined.

WE have previously reported¹ on the structure of plathyterpol but were then unable to define its stereochemistry. An X-ray analysis of a derivative of the terpene together with o.r.d. measurements performed by Professor Klyne now enables us to define plathyterpol as (I), which in particular, confirms our previous tentative suggestion that the compound has the unusual A: B-cis-ring fusion. Plathyterpol thus differs from its stereoisomer, kolavelool² (II), at two centres, at least.

We have been unable to prepare a crystalline derivative of plathyterpol still containing the original asymmetry at C-13 so the stereochemistry at that point remains unknown. However the dibromo-ketone (III) prepared by ozonolysis of dibromoplathyterpol crystallised well and proved suitable for X-ray structure analysis.

The cell parameters were established as:—Space group $P2_1$, $a = 11.91 \pm 0.02$, $b = 7.71 \pm 0.01$, $c = 10.00 \pm 0.02$ Å, $\beta = 92^{\circ} 53' \pm 6'$, U = 917 Å³, $D_{\rm m} = 1.523$, Z = 2, $D_{\rm c} = 1.540$.

Intensity measurements were made on a Hilger and Watts linear diffractometer using $Mo-K_{\alpha}$ radiation with the crystal mounted so as to rotate about its axis b. 1324 reflections, measured from the layers h0l-h9l, were used in structure determination by the heavy-atom method. A

three-dimensional Patterson synthesis and successive structure factor calculations and Fourier syntheses lead to



the structure (III) and this was confirmed by full-matrix least-squares refinement. The final R value was 9.0%.

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(II)

¹ T. J. King and S. Rodrigo, Chem. Comm., 1967, 575.

² R. Misra and S. Dev, Tetrahedron Letters, 1968, 2685.