

X-Ray Analysis of the Triterpene Papyriogenin G

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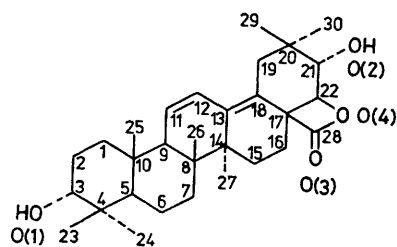
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Summary The new oleanane-type triterpene, papyriogenin G, has been shown by X-ray analysis to have the structure $3\alpha,21\alpha$ -dihydroxyoleana-11,13(18)-diene-22 β ,28-lactone.

ELUCIDATION of the structures of papyriogenin A¹ and papyrioside L-IIa,² which were isolated from the leaves of *Tetrapanax papyriferum* (Araliaceae), has been reported. We report here the crystal structure analysis of a new oleanane-type triterpene, papyriogenin G, obtained from ether extracts of the leaves of same plant; m.p. 188–190 °C; ν_{\max} (KBr) 1828 cm⁻¹; λ_{\max} 248, 256, and 264 nm (heteroannular diene); diacetate, m.p. 193–195 °C; ν_{\max} 1822 and 1732 cm⁻¹. The structure of papyriogenin G could be tentatively assigned by comparison of its spectral data with data for papyriogenin A, but to determine its structure unambiguously, an X-ray study was undertaken.



Papyriogenin G

Crystal data: papyriogenin G, C₃₀H₄₄O₄, space group *P*2₁2₁2₁, orthorhombic, with *a* = 14.994, *b* = 22.272, *c* = 7.656 Å, *Z* = 4.† Intensity data were collected using Cu-K α radiation on an automatic four-circle diffractometer and 2986 independent reflections were recorded. The

† The atomic co-ordinates for this work are available on request from the Director of the Cambridge Crystallographic Data Centre, University Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW. Any request should be accompanied by the full literature citation for this communication.

structure was solved by direct methods using the program MULTAN.³ Block-diagonal least-squares refinement with anisotropic temperature factors for C and O converged at an *R* value of 0.094 for 2510 reflections with $|F_o| \geq 2\sigma(F_o)$.

The structure is fully consistent with the spectral and chemical data. In particular, the β -lactone bridge between

C-28 and C-22 explains the unusually high frequency of the CO absorption at 1828 cm⁻¹. Papyriogenin G is the first example of a naturally occurring triterpenes, having a four-membered lactone ring.

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¹ S. Amagaya, M. Takai, Y. Ogihara, and Y. Iitaka, *J.C.S. Chem. Comm.*, 1975, 991; S. Amagaya, M. Takai, Y. Ogihara, and Y. Iitaka, *Acta Cryst.*, 1977, **33**, 261.

² M. Takai, S. Amagaya, and Y. Ogihara, *J.C.S. Perkin I*, 1977, 1801.

³ P. Main, M. M. Woolfson, and G. Germain, MULTAN, a Computer Program for the Automatic Solution of Crystal Structures, Universities of York and Leuven, 1971.