Base R, the *X*-Ray Crystal Structure of a Novel Lycopodium Alkaloid

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Summary The crystal structure of the novel alkaloid Base R reveals its relation to fawcettidine.

ONE of the minor bases from *Lycopodium fawcettii*, called Base R was shown to have molecular formula $C_{16}H_{24}N_2O_2$, a five-membered ring ketone and hydroxy and secondary amino-groups, and only one methyl residue.[1] We now report its *X*-ray crystal structure.

The perchlorate salt was selected and this crystallises in the orthorhombic space group $C222_1$ (D_2^5, No. 20) with $a = 15{\cdot}65$, $b = 8{\cdot}40$, and $c = 25{\cdot}35$ Å, $C_{16}H_{24}N_2O_2{\cdot}HClO_4$, $M = 406{\cdot}5$, $Z = 8$, $D_m = 1{\cdot}51$, $D_c = 1{\cdot}497$ g cm^{-3}.

The intensity data were recorded on a Picker four-circle diffractometer using Mo-K_α radiation. Normalized structure factors were computed and the structure solved by direct methods using the program MULTAN.[2] Two perchlorate anions were thus revealed to occupy the special positions of the group. Three atoms missing in the original E map and twenty three H atoms were afterwards located by difference Fourier synthesis. The model was refined by least-squares to a R value of 8·6% using isotropic temperature factors for all atoms. Consideration of the behaviour of the B's during refinement permitted the determination of the positions of the cation nitrogen and oxygen atoms (Figure).

This pentacyclic structure, (**1**), in the normal Lycopodium convention, is closely related to and biogenetically compatible with other alkaloids, such as fawcettidine (**2**) (also found in this plant). An inversion of the configuration at C(4) (adjacent to the carbonyl) is necessary for insertion of the –NH– bridge between C(5) and C(13). From the o.r.d. data ($[\alpha]_D + 104°$, $[\alpha]_{312} + 1870°$, $[\alpha]_{270} -1730°$: positive Cotton effect) the absolute stereochemistry must be as shown.

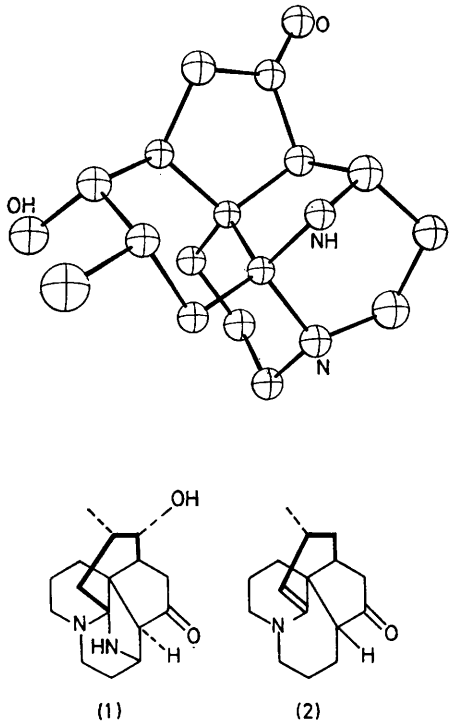

FIGURE. Crystal structure of Base R.

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[1] R. H. Burnell, C. G. Chin, B. S. Mootoo, and D. R. Taylor, *Canad. J. Chem.*, 1963, **41**, 3091.
[2] G. Germain, P. Main, and M. H. Woolfson, *Acta Cryst.*, 1970, **B26**, 274.