

S(+)-MAGNOFLORINE BROMIDE: ISOLATED FROM CROTON TURUMIQUIRENSIS

R. H. BURNELL and A. CHAPELLE

Département de Chimie, Université Laval, Québec, Canada

P. H. BIRD

Chemistry Department, Concordia University, Montréal, Canada

Previous difficulties in isolating pure quaternary alkaloids from Venezuelan *C. turumiquirensis* (1) prompted us to approach the identification of the bases by X-ray diffraction. After the anion was exchanged from chloride to bromide, a sample of one of the quaternary salts was crystallized from methanol by slow diffusion of acetone. The mother liquors darkened somewhat, but a small quantity of an alkaloid bromide appeared as well-formed prisms.

Monoclinic, prismatic b, C₂ (C₂³), a=24.17, b=8.31, c=11.60 Å, β=109° 30'. C₂₀H₂₆N₄Br·CH₃OH, F.W. 456.4, Z=4.

The space group was determined from systematic absences by Weissenberg, and precession photographs and intensities were measured on a fully automated Picker four-circle diffractometer. Fourier and least-squares

methods afforded structure 1, which is that of magnoflorine bromide (2). A molecule of methanol of crystallization also became apparent during refinement.

The diphenyl system in the aporphine series of alkaloids cannot assume planarity, and, in the case of magnoflorine, the results show a dihedral angle of 29° between the planes of the aromatic rings. The molecule is, of course, optically active; from the positive Cotton effect in the optical rotatory dispersion (3), the Croton base is shown to be S(+)-magnoflorine bromide, mp 220° (decomp.), [α]²⁰_D+222° (EtOH). The final value of R is 0.14. Although this is the first alkaloid identified in the species, no further work is planned on the crystal because it is a known compound. Full details of this work are available (4).

Experimental conditions. Source MoKα, λ=0.7107 Å, 943 non-zero independent reflections.

Received 25 June 1980

LITERATURE CITED

1. R. H. Burnell and D. Della Casa, *Nature*, **203**, 296 (1964).
2. M. Shamma and W. A. Slusarchyk, *Chem. Reviews*, **64**, 59 (and references cited therein) (1964).
3. J. Cymerman-Craig and S. K. Roy, *Tetrahedron*, **21**, 395 (1965).
4. A. Chapelle, Graduate Thesis, Université Laval, Québec, Canada (1974).

