Structure of Tropane Alkaloids from Rotational Spectra: Scopine vs Scopoline

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Tropane alkaloids are chemicals producing different pharmacological effects, which share a characteristic eight-membered aza-bicyclic motif. Following an initial study of tropinone ($C_8H_{13}NO$) [1] we report here the analysis of the conformational properties of the epoxytropane scopine ($C_8H_{13}NO_2$) using Fourier-transform microwave (FT-MW) spectroscopy in a supersonic jet expansion.

Scopine was initially vaporized using conventional heating methods at moderate temperatures below 100ºC. However, the rotational spectrum was not compatible with any conformation of scopine, eventually resulting in the assignment of the structural isomer of scopoline (Fig. 1). In scopoline an intramolecular reaction breaks the epoxy group, seriously distorting the tropane ring [2] and inverting the *N*-methyl group.

In order to observe scopine we then turned to laser vaporization techniques using a ps YAG laser. The rotational spectrum now yielded no traces of scopoline and scopine was finally assigned. Following long scans in the 6-18 GHz cm-wave region a single conformer for the molecule was detected. Rotational constants, centrifugal distortion corrections and ^{14}N nuclear quadrupole coupling hyperfine parameters will be reported for scopine. The intramolecular effects controlling the axial/equatorial equilibrium of the *N*-methyl group will be additionally discussed.

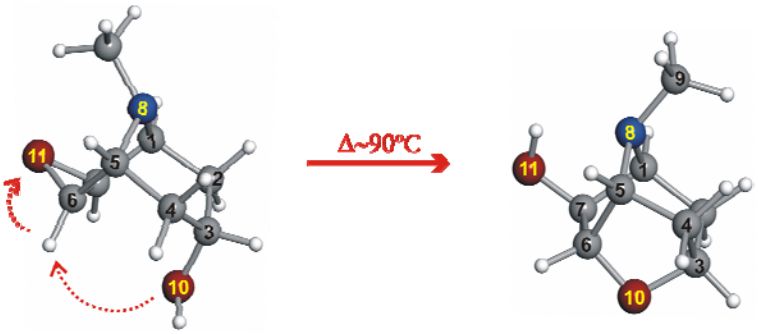

Figure 1. Intramolecular gas-phase rearrangement of scopine (left) into scopoline. The thermal reaction can be prevented using laser vaporization.

[1] E. J. Cocinero, A. Lesarri, P. Écija, J.-U. Grabow, J. A. Fernández, F. Castaño, *Phys. Chem. Chem. Phys.* **2010**, *12*, 6076.
[2] P. Écija, E. J. Cocinero, A. Lesarri, F. J. Basterretxea, J. A. Fernández, F. Castaño, *Chem. Phys. Chem.* **2013**, *14*, 1830.