ROTATIONAL INVESTIGATION OF TROPANE ALKALOIDS

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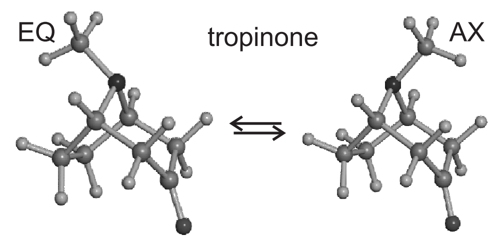

We report an investigation of the rotational spectrum of several tropane alkaloids using the new Balle-Flygare-type FT-MW spectrometer[a] built at the University of the Basque Country. The initial work focused on the azabicycles of tropinone, scopine and scopoline, vaporized using heating methods. For tropinone[b] the spectrum confirmed the presence of equatorial and axial conformers originated by the inversion of the *N*-methyl group, with the tropane motif adopting a distorted chair configuration. The determination of substitution and effective structures for the two conformers included the ^{13}C, ^{15}N and ^{18}O isotopomers observed in natural abundance. The structures revealed the flexibility and structural changes associated to the *N*-methyl inversion, mostly a flattening at the nitrogen atom and a simultaneous rising of the carbonyl group in the axial form. The investigation of scopine gave an intense spectrum, but it was inconsistent with the structural models expected for this molecule. The carrier of the new spectrum was later identified as scopoline, generated *in situ* by an intramolecular reaction at the moderate temperatures of the nozzle. A single conformation was detected for scopoline, with an ether bridge seriously distorting the tropane motif.

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[a] E. J. Cocinero, A. Lesarri, P. Écija, J.-U. Grabow, J. A. Fernández, F. Castaño, in publication, 2010

[b] E. J. Cocinero, A. Lesarri, P. Écija, J.-U. Grabow, J. A. Fernández, F. Castaño, *Phys. Chem. Chem. Phys.*,in press, 2010