UNRAVELLING THE CONFORMATIONAL LANDSCAPE OF NICOTINOIDS: THE STRUCTURE OF COTININE BY BROADBAND ROTATIONAL SPECTROSCOPY

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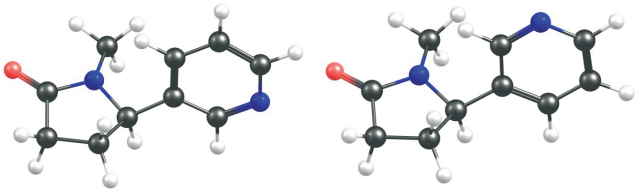

Alkaloids such as nicotine, cotinine or anabasine share a common floppy structural motif consisting of a two-ring assembly with a 3-pyridil methylamine skeleton. In order to investigate the structure-activity relationship of these biomolecules, structural studies with rotational resolution have been carried out for nicotine[a] and anabasine[b] in the gas phase, where these molecules can be probed in an "interaction-free" environment (no solvent or crystal-packing interactions).

We hereby present a structural investigation of cotinine in a jet expansion using the chirped-pulse Fourier-transform microwave (CP-FTMW) spectrometer recently built at the University of the Basque Country (UPV-EHU). The rotational spectrum (6-18 GHz) reveals the presence of two different conformations. The conformational preferences of cotinine originate from the internal rotation of the two ring moieties, the detected species differing in a near 180° rotation of pyridine. The final structure is modulated by steric effects.

[a] J.-U. Grabow, S. Mata, J. L. Alonso, I. Peña, S. Blanco, J. C. López, C. Cabezas, *Phys. Chem. Chem. Phys.* 2011, **13**, 21063.
[b] A. Lesarri, E. J. Cocinero, L. Evangelisti, R. D. Suenram, W. Caminati, J.-U. Grabow, *Chem. Eur. J.* 2010, **16**, 10214.