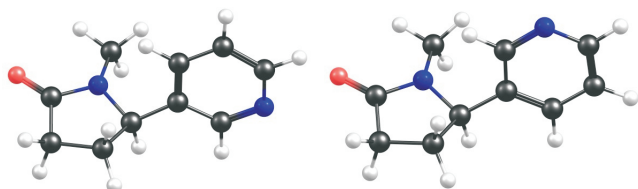


UNRAVELLING THE CONFORMATIONAL LANDSCAPE OF NICOTINOIDS: THE STRUCTURE OF COTININE BY BROADBAND ROTATIONAL SPECTROSCOPY

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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.

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^bA. Lesarri, E. J. Cocinero, L. Evangelisti, R. D. Suenram, W. Caminati, J.-U. Grabow, *Chem. Eur. J.* 2010, **16**, 10214.