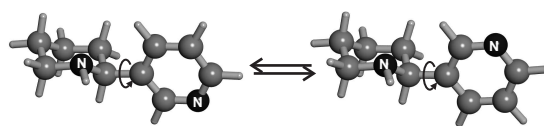


CONFORMATIONAL LANDSCAPE OF NICOTINOIDS: SOLVING THE "CONFORMATIONAL DISPARITY" OF ANABASINE

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The conformational landscape of the alkaloid anabasine (neonicotine) has been investigated using rotational spectroscopy and *ab initio* calculations. The results allow a detailed comparison of the structural properties of the prototype piperidinic and pyrrolidinic nicotinoids (anabasine vs. nicotine^a). Anabasine adopts two most stable conformations in isolation conditions, for which we determined accurate rotational and nuclear quadrupole coupling parameters. The preferred conformations are characterized by an equatorial pyridine moiety and additional N-H equatorial stereochemistry at the piperidine ring (*Eq-Eq*). The two rings of anabasine are close to a bisecting arrangement, with the observed conformations differing in a ca. 180° rotation of the pyridine subunit, denoted either *Syn* or *Anti*. The preference of anabasine for the *Eq-Eq-Syn* conformation has been established by relative intensity measurements (*Syn/Anti*~5(2)). The conformational preferences of free anabasine are directed by a N···H-C weak hydrogen bond interaction between the nitrogen lone pair at piperidine and the closest hydrogen bond in pyridine, with N···N distances ranging from 4.750 Å (*Syn*) to 4.233 Å (*Anti*).



^aR. J. Lavrich, R. D. Suenram, D. F. Plusquellic and S. Davis, 58th OSU Int. Symp. on Mol. Spectrosc., Columbus, OH, 2003, Comm. RH13