

¹⁴N NUCLEAR QUADRUPOLE HYPERFINE STRUCTURE AND LARGE AMPLITUDE MOTIONS IN 2-METHYL-2-IMIDAZOLINE STUDIED BY ROTATIONAL SPECTROSCOPY

KATEŘINA LUKOVÁ, LUCIE KOLESNIKOVÁ, KAREL VÁVRA, PATRIK KANIA, RADIM NESVADBA, *Department of Analytical Chemistry, Institute of Chemical Technology, Prague, Czech Republic*; JAN KOUCKÝ, *Analytical Chemistry, Institute of Chemical Technology, Prague, Praha 6, Czech Republic*; ZBIGNIEW KISIEL, *ON2, Institute of Physics, Polish Academy of Sciences, Warszawa, Poland*; STEPAN URBAN, *Department of Analytical Chemistry, Institute of Chemical Technology, Prague, Czech Republic*.

2-methyl-2-imidazoline, also known as lysidine, is a non-planar heterocyclic molecule containing two ¹⁴N quadrupolar nuclei and one methyl group. The rotational spectra of this molecule were recorded in the frequency range from 7 to 20 GHz using a pulsed molecular jet Fourier transform microwave spectrometer^a and in selected frequency regions between 90 and 220 GHz using two different millimetre-wave spectrometers^{b,c}. Lysidine displays a very rich millimetre wave spectrum presumably attributable to the presence of two large amplitude motions in the molecule: an internal rotation of the methyl group and a ring-puckering motion. The decimetre-wave spectra are even more complex as the hyperfine structure arising from the nuclear quadrupole coupling interactions of two ¹⁴N nuclei is also resolved. The first analysis of this challenging spectrum guided by quantum chemical calculations is reported in the present contribution.

^aV. Kabourek, P. Černý, P. Piksa, T. Studecký, P. Kania, Š. Urban, *Radioengineering*, 22, (2013), 1288–1295.

^bP. Kania, L. Střiteská, M. Šimečková, Š. Urban, *J. Mol. Struct.*, 1–3, (2006), 209–218.

^cZ. Kisiel, A. Kraśnicki, *J. Mol. Spectrosc.*, 262, (2010), 82–88.