THE JET-COOLED ROTATIONAL SPECTRUM OF GLYCINAMIDE, AN AMINOACID PRECURSOR

ELENA R. ALONSO, LUCIE KOLESNIKOVÁ, Grupo de Espectroscopia Molecular, Lab. de Espectroscopia y Bioespectroscopia, Unidad Asociada CSIC, Universidad de Valladolid, Valladolid, Spain; ZBIGNIEW KISIEL, ON2, Institute of Physics, Polish Academy of Sciences, Warszawa, Poland; J.-C. GUILLEMIN, UMR 6226 CNRS - ENSCR, Institut des Sciences Chimiques de Rennes, Rennes, France; JOSÉ L. ALONSO, Grupo de Espectroscopia Molecular, Lab. de Espectroscopia y Bioespectroscopia, Unidad Asociada CSIC, Universidad de Valladolid, Valladolid, Spain.

The glycinamide H₂NCH₂CONH₂, considered as one of the possible precursors of glycine, has been generated in the gas phase via laser ablation of glycinamide hydrochloride. The vaporized products were seeded in neon, expanded adiabatically into the vacuum chamber of the spectrometer and probed by broadband chirped pulsed Fourier transform microwave spectroscopy. The most stable conformer is stabilized by an intramolecular hydrogen bonding interaction between the lone pair on the nitrogen in the amine group and the H-N bond in the amide group was observed in accordance with the previous millimeter wave study ^a. Glycinamide possesses two ¹⁴N nuclei with a nuclear quadrupole moment I=1, which give rise to a complex hyperfine structure. We took advantage of the higher resolution of our narrowband LA-MB-FTMW spectrometer ^b to fully resolve the nuclear quadrupole hyperfine structure. More than 90 nuclear quadrupole hyperfine components belonging to 5 different rotational transitions were analyzed. This provides a definitive evidence to establish the most stable observed conformer.

^aZ.Kisiel, E.Białkowska-Jaworska, L.Pszczółkowski, J.C.Guillemin, 21st HRMS, Poznań, 2010.

^bC.Bermudez, S. Mata, C.Cabezas, and J.L.Alonso, Angew. Chem. 2014, 126, 11195–11198.