ROTATIONAL SPECTRA AND MOLECULAR CONFORMATION OF TWO CONFORMERS OF LEUCINAMIDE

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The rotational spectra of the parent species of two conformers of the amino acid derivative leucinamide have been recorded between 10.5 and 20 GHz using a Balle-Flygare Fourier-transform microwave spectrometer. 6 *a*- and *b*-type rotational transitions were recorded for conformer I and 23 *a*- and *b*-type rotational transitions were recorded for conformer II. The rotational constants are $A = 2274.94(9)$ MHz, $B = 1033.336(7)$ MHz, and $C = 911.732(3)$ MHz and $A = 2752.775(8)$ MHz, $B = 843.502(1)$ MHz, and $C = 796.721(1)$ MHz for conformers I and II respectively. The congested hyperfine patterns arising from the two ^{14}N nuclei were not resolved. Comparison of the experimental moments of inertia to those derived from the lowest energy ab initio (MP2/6-311++G(d,p)) structures indicates gas-phase backbone structures that differ from both the crystal structures of leucinamide[a] and the gas-phase structures of the amino acid leucine[b].

[a] P. Belton and Y. Wang, *J. Mol. Struct.*, *602-603*, 2002, 71-78.

[b] E. J. Cocinero, A. Lesarri, J.-U. Grabow, J. C. López, and J. L. Alonso, *ChemPhysChem*, *8*, 2007, 599-604.