MOLECULAR CONFORMATION OF THE AMINO ACID DERIVATIVE ALANINAMIDE

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We report the rotational spectra of alaninamide and two ^{15}N labeled isotopomers. The derived rotational constants of the most abundant isotopomer are A = 4931.924 (2) MHz, B = 3114.594 (2) MHz, and C = 2297.252 (2) MHz. Fifty-two hyperfine components associated with 3 *a*-type and 3 *b*-type transitions were fit yielding quadrupole coupling constants of χ_{aa} = 1.603 (4) MHz and χ_{bb} = 0.643 (6) MHz for the amino nitrogen and χ_{aa} = 1.379 (5) MHz and χ_{bb} = 0.570 (6) MHz for the amide nitrogen. A preliminary Kraitchman calculation indicates a nitrogen-to-nitrogen distance of 2.803 Å, suggesting that the experimentally determined conformer contains an intramolecular hydrgoen bond from the amide nitrogen to the amino nitrogen.