ROTATIONAL SPECTRUM AND STRUCTURE OF A VAN DER WAALS COMPLEX BETWEEN AN AMINO ACID DERIVATIVE AND WATER: ALANINAMIDE - H_2O

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The structure of the amino acid derivative alaninamide was determined by substitution of all the heavy atoms except oxygen. Assignment of the rotational spectrum of the 1:1 complex of alaninamide and water yielded rotational constants for the most abundant isotopomer: A = 4789 (3) MHz, B = 1271.872 (8) MHz, and C = 1111.394 (8) MHz. Preliminary data from two ^{15}N isotopomers indicate that the conformation of the alaninamide monomer is relatively unchanged upon complexation and that the water complex has a cyclic hydrogen bonded network, in which the water interacts with the carbonyl oxygen and an amide hydrogen.