Ψ AND Φ DIHEDRAL CONFORMATIONAL ANGLES FOR THE DIPEPTIDE MIMETIC: ETHYL ACETAMIDOACETATE ($CH_3CONHCH_2COOCH_2CH_3$)

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The microwave spectrum of the glycine amino-acid derivative, ethyl acetamidoacetate ($CH_3CONHCH_2COOCH_2CH_3$), has been recorded with a pulsed-molecular-beam Fourier-transform microwave spectrometer. This compound was chosen for study since it possesses peptide-like dihedral conformation angles Φ and Ψ responsible for the flexibility of polypeptide and protein amino acid chains. The microwave spectrum provides information on the values of these angles for the conformers which are populated at the approximately 2 K rotational temperature of the supersonic expansion. In contrast to most dipeptides, the melting point of the ethyl acetamidoacetate is low enough that sufficient vapor pressure of the compound can be achieved at temperatures near 400 K without competition from decomposition. At present, rotational transitions have been measured for only the lowest energy conformer of this dipeptide mimetic. Both a- and b-type rotational transitions are observed, with the K = 0 transitions being split by approximately 25 MHz due to methyl top internal rotation. Each internal rotation component is further split on the order of 1 MHz by the nuclear quadrupole interaction of the I=1 ^{14}N quadrupolar nucleus. The rotational constants, A= 4411.28991(87) MHz, $B + C$ = 933.00329(68) MHz, and $B - C$ = 43.94339(93) MHz and nuclear quadrupole hyperfine constants eQq_{aa} = 2.285(32) MHz and eQq_{bb} = 5.954(38) MHz have been determined. Attempts are presently underway to identify other conformers in the molecular beam and to determine the geometry of the conformer observed.