MOLECULAR CONFORMATION OF METHAMPHETAMINE

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We report the rotational spectrum of the normal species of methamphetamine and its ^{15}N isotopomer. For the normal isotopomer, A = 2121.7117(7) MHz, B = 613.2416(1) MHz, and C = 575.5221(2) MHz. Assignment of the resulting nuclear quadrupole hyperfine structure for the normal species results in, χ = 1.080(4) MHz and χ_{bb} = 2.623(2) MHz. Ongoing ab initio calculations at the MP2/6-31G(d,p) level have resulted in six minima on the potential energy surface. In these calculations, the lowest energy conformations have the amide proton oriented towards the phenyl ring. Coordinates of the nitrogen atom calculated from a preliminary least-squares-fit of the microwave data and subsequent Kraitchman analysis are in good agreement with one another and are consistent with the lowest energy ab initio structure.