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ABSTRACT

Rotational spectra of the most abundant and four ^{13}C isotopomers of 4-aminobutanol have been recorded in natural abundance using a Fourier-transform microwave spectrometer. For the most abundant isotopomer, 56 hyperfine components from the fifteen a- and b-type transitions measured were fit to the quadrupole coupling constants, χ_{aa} = -3.843(3) MHz, χ_{bb} = 1.971(3) MHz. Rotational and centrifugal distortion constants determined from fits of the resulting unsplit line centers to the Watson A-reduction Hamiltonian are A=4484.893(3) MHz, B= 2830.721(1) MHz, C= 1942.9710(3) MHz, Δ_J = 0.98(3) kHz, Δ_{JK}= 1.4(1) kHz, Δ_K = -2.6(5) kHz, δ_J = 0.27(1) kHz, and δ_K = 1.7(1) kHz. Between nine and eleven rotational transitions were measured for the ^{13}C isotopes and rotational constants were determined by fixing the distortion constants to the values found for the normal isotope. The five sets of moments of inertia were used to determine the 4-aminobutanol substitution structure as well to perform a least-squares fit of the lowest energy ab initio structure. The heavy atom coordinates determined from these two methods are in excellent agreement. The conformation of 4-aminobutanol is stabilized by an intramolecular hydrogen bond from the alcohol proton to amino nitrogen with a resulting hydrogen bond distance of 1.891 Å. The experimental structure is consistent with the lowest energy ab initio [MP2/6-311++G(d,p)] structure.