CONFORMATIONAL ANALYSIS OF VALINE METHYL ESTER BY MICROWAVE SPECTROSCOPY

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The rotational spectra of two conformers of valine methyl ester (ValOMe) have been measured and assigned using a cavity based Fourier-transform microwave spectrometer in the range of 9-18 GHz as a part of a project investigating the structures of a series of amino acid methyl esters. We modeled 15 possible conformers of ValOMe using the ωB97XD/6-311++G(d,p)) level of theory. 59 rotational transitions assigned to conformer I were fit to Watson's *A*-reduced Hamiltonian: A = 2552.01(1) MHz, B = 1041.821(2) MHz, and C = 938.549(2) MHz. ^{14}N nuclear quadrupole hyperfine splittings were resolved, and the 137 hyperfine components were fit to χ_{aa} = -4.20(2) MHz and $\chi_{bb} - \chi_{cc}$ = 1.26(1) MHz. The spectrum of conformer I also reveals tunneling splittings from the ester methyl rotor. The *XIAM*[a] program was used to fit the barrier to the internal rotation of the methyl rotor. The best fit V_3 barrier was found to be 387.8(8) cm^{-1}. 20 rotational transitions were assigned for conformer II and the fitted rotational constants are A = 2544.405(9) MHz, B = 1092.337(2) MHz, and C = 896.301(1) MHZ. The transitions were split by nuclear quadrupole coupling and tunneling, and complete assignment of these components is ongoing.

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[a]H. Hartwig and H. Dreizler, Z. Naturforsch. **51a**, (1996) 923.