ROTATIONAL SPECTRA OF THE ANTI-ANTI CONFORMER OF N-BUTYLGERMANE

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Rotational spectra for the five naturally occurring germanium isotopologues of the anti-anti conformer of n-butylgermane have been measured using a Fourier-transform microwave spectrometer operating in the 4-18 GHz range. This conformer, determined by ab initio calculations at the MP2/6-311++G(2d,2p) level to be the most stable of five possible conformers, has a heavy atom planar structure and dipole moment values (for the ^{74}Ge species) of $\mu_a = 0.7332(85)$ D and $\mu_b = 0.489(46)$ D, with $\mu_{\mathrm{total}} = 0.881(26)$ D.
Nuclear quadrupole coupling constants have also been determined for the $I = 9/2$ ^{73}Ge nucleus and are in reasonable agreement with ab initio calculations. Small splittings, which were particularly apparent on the very weak b-type transitions for all isotopic species, are presumably due to rotation of one or both of the internal rotors (CH_3 and GeH_3) although these splittings have not yet been resolved sufficiently well to allow determination of any internal rotation parameters. The spectroscopic data will be discussed in relation to ab initio results and compared with results for similar species.