ROTATIONAL SPECTRA OF CYCLOPROPYLMETHYL GERMANE AND CYCLOPROPYLMETHYL SILANE: DIPOLE MOMENT AND BARRIER TO METHYL GROUP ROTATION

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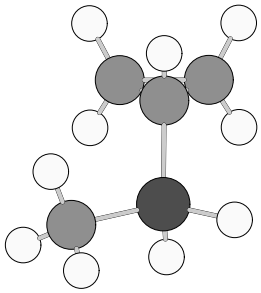

The Fourier-transform microwave spectra corresponding to the gauche conformer of five isotopologues of cyclopropylmethyl germane and three isotopologues of cyclopropylmethyl silane have been assigned. *a*-, *b*- and *c*-type transitions are all split into doublets by internal rotation of the methyl group; a global fit of the *A* and *E* state spectra leads to barriers to rotation of 4.736(6) kJ mol^{-1} in the germane and *ca.* 6.7 kJ mol^{-1} in the silane. Stark effect measurements reveal similar dipole moment components for both molecules: $\mu_a = 0.1782(10)$ D, $\mu_b = 0.581(4)$ D, $\mu_c = 0.305(9)$ D and $\mu_{\mathrm{total}} = 0.680(5)$ D for the germane and preliminary values of $\mu_a = 0.196(4)$ D, $\mu_b = 0.670(5)$ D, $\mu_c = 0.363(8)$ D and $\mu_{\mathrm{total}} = 0.787(6)$ D for the silane.

Nuclear quadrupole coupling constants for the ^{73}Ge isotopologue ($I = \frac{9}{2}$) of cyclopropylmethyl germane have been determined and are in good agreement with values predicted at the B3LYP/6-311++G(3df,3pd) level. The electric field gradient at the Ge nucleus will be compared with related germanes and the barriers to rotation for both the germane and the silane will be compared with similar species.