PECULIAR TRAITS OF HSOH IN ITS ROTATIONAL-TORSIONAL SPECTRUM ABOVE 1 THz

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In this paper we present highly accurate spectral data of oxadisulfane, HSOH, in the region of 1.1–1.3 THz. The simple skew chain molecule HSOH is an asymmetric rotor close to the limiting case of a symmetric prolate top molecule. Therefore the pure rotational spectra of this molecule appear very simple at first glance. However, if the spectra are inspected in detail, the molecule manifests its peculiarities.

HSOH can be considered as a link between the well-known molecules HSSH and HOOH. For these two species a simple model to explain the alternation of the torsional splittings with the rotational quantum number K_a has been proposed by Hougen[a]. HSOH obviously has lower symmetry than HSSH and HOOH and therefore the observed variation of the torsional splittings with the rotational quantum number K_a cannot be explained by the Hougen model. The new data allow to calculate the experimental tunneling splitting of energy levels up to K_a=7 for the first time. The obtained results are essential to test novel models[b,c,d] on torsional tunneling splitting in HSOH.

In case of $K_a'' < 3$ the HSOH molecule displays a dominating perpendicular-type spectrum in the vibrational ground state with strong c- and somewhat weaker accompanying b-type transitions, as can be understood from theoretical values of the dipole-moment components. In contrary, transitions with $K_a'' \geq 3$ display only c- but no b-type transitions. The absence of b-type transitions is completely unexpected and yet not well understood.

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