FOURIER TRANSFORM MICROWAVE SPECTRA OF 1-PENTANETHIOL-*d*

NOBUHIKO KUZE, YOSHIYUKI KAWASHIMA, *Department of Materials and Life Sciences, Sophia University, Tokyo, Japan*.

We have been observing the rotational spectra of the 1-pentanethiol (1-C_5SH; C(5)H_3C(4)H_2-C(3)H_2C(2)H_2C(1)H_2SH) by Fourier transform microwave (FTMW) spectroscopy. So far, eight conformers of the normal species for 1-C_5SH have been identified by FTMW spectroscopy and the quantum chemical calculations[a]. They are *TTTg*, *TTTt*, *TTGg*, *TTGg'*, *TGTg*, *TGTg'*, *GTTg*, and *GTTg'*. The nomenclature of the conformer such as *TTGg'* is based on the conformation of the molecular skeleton around the C(4)-C(3), C(3)-C(2), C(2)-C(1), and C(1)-S axis, respectively. This means that *TTGg'* represents trans (*T*), trans (*T*), clockwise gauche (*G*) and anti-clockwise gauche (*g'*) conformers.

In this work, we observed the isotopologues the 1-pentanethiol such as the deuterated species in the thiol group, 1-C_5SD. The rotational spectral lines of the seven conformers in 1- C_5SD, except for *TTTt*, were assigned as in 1-C_5SH. In the *TTTg* conformer of 1-C_5SH, characteristic splittings were observed in the rotational spectral lines of the *c*-type transitions. They are due to the tunneling splitting by the torsional motion of the SH group. Therefore, we focused on the line spllitings in the *c*-type transition of the *TTTg* conformer of 1-C_5SD and compared our results with data from 1-C_5SH and related compounds, 1-butanethiol[b], 1-propanethiol and 1-ethanethiol.

[a] K. Suzuki, N. Kuze and Y. Kawashima, ISMS, WI05 (2019).

[b] Y. Kawashima, Y. Tanaka, T. Uzuyama, and E. Hirota, *J. Phys. Chem. A*, 125, 1166-1183 (2021).