CHIRALITY OF AND GEAR MOTION IN ISOPROPYL METHYL SULFIDE: A FOURIER TRANSFORM MICROWAVE STUDY

YOSHIYUKI KAWASHIMA, KEISUKE SAKIEDA, Department of Applied Chemistry, Faculty of Engineering, Kanagawa Institute of Technology, Atsugi, Kanagawa 243-0292, JAPAN; and EIZI HIROTA, The Graduate University for Advanced Studies, Hayama, Kanagawa 240-0193, JAPAN.

Isopropyl methyl sulfide (CH$_3$)$_2$CHSCH$_3$ was investigated by Fourier transform microwave spectroscopy. Two rotational isomers gauche and trans were detected. The rotational spectra of gauche were found fit to an asymmetric rotor pattern, except for being split by the internal rotation of CH$_3$ attached to S with the potential barrier $V_3$ of 601.642 (65) cm$^{-1}$ and for exhibiting the effect of tunneling between the two equivalent gauche forms in a few high-$K$ transitions. The tunneling was discussed from a viewpoint of chirality. The trans spectra appeared generally similar to those of gauche, with $V_3$ to the S-CH$_3$ internal rotation of 559.00 (11) cm$^{-1}$, but satellite lines accompanied the ground torsional state lines in some high-$K$ transitions. These satellites were ascribed to the excited state of the C(isop)-S torsion. In fact, the potential function for this torsion was shown by an ab initio calculation to be flat or even of double minima around the trans position, which was presumably caused by a gear coupling between the two methyl groups of the isopropyl group and the one in the S-CH$_3$. 