

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)₂CHSCH₃ 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 CH₃ 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-CH₃ 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-CH₃.