ISOMERIZATION AMONG THE ISOMERS OF 2-HEXENAL and 3-HEXENAL BY FOURIER TRANSFORM MICROWAVE SPECTROSCOPY

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cis-3-Hexenal (c3H; O = CH – CH2 – CH = CH – CH2 – CH3) is known as a grass odorant molecule, and this compound readily isomerizes to trans-2-hexenal (t2H). We have previously identified two conformers of c3H by Fourier transform microwave (FTMW) spectroscopy [1]. We also found the isomers of c3H, trans-3-hexenal (t3H) and cis-2-hexenal (c2H), from rotational spectra observed on liquid sample of c3H. In this study, the intensities of the rotational spectral lines of these conformers of 3- and 2-hexenal were measured repeatedly to obtain reliable temperature-dependent intensity ratio profiles of the isomerization reactions. The rotational spectra of c3H and t3H were observed at 30:1 in the first step in room temperature. The t3H isomer was found to be contained in the liquid c3H sample as an impurity. As the nozzle temperature was increased, the line intensities of the t2H and c2H became stronger, and finally, the ratio of t2H and c2H was 6:1. This indicates that c3H may isomerize to both t2H and c2H. We also discuss the identification of the second conformer for c3H; the structural model in which all dihedral angles of the C-C single bond are in the skew configuration, SScS, is better than the previously identified conformer [1], CScS, in which the OCCC dihedral angle is in the cis configuration.