

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

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cis-3-Hexenal (*c*3H; $O = CH - CH_2 - CH = CH - CH_2 - CH_3$) is known as a grass odorant molecule, and this compound readily isomerizes to *trans*-2-hexenal (*t*2H). We have previously identified two conformers of *c*3H by Fourier transform microwave (FTMW) spectroscopy [1]. We also found the isomers of *c*3H, *trans*-3-hexenal (*t*3H) and *cis*-2-hexenal (*c*2H), from rotational spectra observed on liquid sample of *c*3H. 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 *c*3H and *t*3H were observed at 30:1 in the first step in room temperature. The *t*3H isomer was found to be contained in the liquid *c*3H sample as an impurity. As the nozzle temperature was increased, the line intensities of the *t*2H and *c*2H became stronger, and finally, the ratio of *t*2H and *c*2H was 6:1. This indicates that *c*3H may isomerize to both *t*2H and *c*2H. We also discuss the identification of the second conformer for *c*3H; 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.

[1] R.Ozawa, N. Kuze and Y. Kawashima, *ISMS*, P6243 (2022).