

FOURIER TRANSFORM MICROWAVE SPECTRA OF *cis*-3-HEXENAL, *trans*-3-HEXENAL, *cis*-2-HEXENAL AND *trans*-2-HEXENAL: STRUCTURAL ISOMERS AND ISOMERIZATION

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cis-3-Hexenal (*c3*-HA; O=CH-CH₂-CH=CH-CH₂-CH₃) is known as an odor molecule of grass and the *c3*-HA easily isomerizes to *trans*-2-hexenal (*t2*-HA). Rotational spectra of the *c3*-HA and its structural isomers were observed by Fourier transform microwave (FTMW) spectroscopy in the frequency region 4.8-23 GHz. We reported that two conformers of the *c3*-HA, *SG'cS* and *CScS*, were assigned^a: in *SG'cS*, *S*, *G'*, *c*, and *S* in order denote the *skew*, *gauche'*, *cis* and *skew* around the dihedral angles OC(1)C(2)C(3), C(1)C(2)C(3)=C(4), C(2)C(3)=C(4)C(5) and C(3)=C(4)C(5)C(6), respectively. We found other four conformers which were assigned to the *SStS* and *S'S'tS* conformers of *trans*-3-hexenal (*t3*-HA), and the *TcSG'* and *TcST* conformers of *cis*-2-hexenal (*c2*-HA) by comparing from the results of ab initio calculation. We also observed the rotational spectra of the *t2*-HA which had been reported in 2015^b. The spectra of the *c3*-HA and *t3*-HA were observed in room temperature. When the nozzle temperature increased, the maximum of spectral intensities of the *c3*-HA and *t3*-HA reach at around 350 K while the intensities of the *t2*-HA and *c2*-HA are stronger. This evidence shows that the *c3*-HA and *t3*-HA isomerized into the *t2*-HA and *c2*-HA.

^aS. Yoshizawa, N. Kuze and Y. Kawashima, ISMS2019, P3866 (2019).

^bR. Yokoyama, Y. Kawashima, and E Hirota, 9th Annual Meeting on Molecular Science, Tokyo, 4P008 (2015).