CONFORMATIONAL ISOMERISM IN 1-HEPTANAL

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The rotational spectrum of 1-heptanal (CH_3-CH_2-CH_2-CH_2-CH_2-CH_2-CH=O) has been recorded over the 10 GHz to 22 GHz region using a pulsed-molecular-beam, Fourier transform microwave spectrometer. The spectrum has been analyzed using the jb95[1] spectral analysis program. The spectra of thirteen conformational isomers have been identified and assigned in the rich soup of observed transitions. Transitions of these isomers have relative intensities that are well above the intensity level of the onset of ^{13}C isotopomers, which are a factor of 100 down in intensity. In addition to the above 13 isomers, two additional spectra were identified and assigned that belong to dimers that consist of 1-heptanal and one water molecule. In order to map the observed spectra to conformational geometries, high-level *ab initio* calculations have been carried out. All fifteen observed conformers have been associated with *ab initio* determined structure configurations. In general, the agreement in rotational constants and dipole intensity pattern between the *ab initio* results and the experimentally observed spectra is quite good.

[1] http://physics.nist.gov/Divisions/Div844/facilities/uvs/jb95userguide.htm