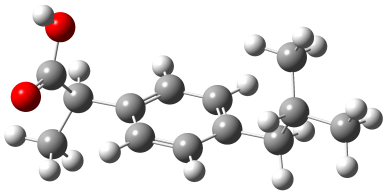
CONFORMATIONAL ANALYSIS OF IBUPROFEN USING BROADBAND MICROWAVE SPECTROSCOPY

SABRINA ZINN[a], THOMAS BETZ, MELANIE SCHNELL, *CoCoMol, Max-Planck-Institut für Struktur und Dynamik der Materie, Hamburg, Germany*.



The broadband rotational spectrum of ibuprofen ((RS)-2-(4-isobutylphenyl)-propanoic acid), a well-known drug, will be presented. As it is used to relieve pain, reduce fever, and inhibit inflammation, the knowledge of its biological activity is very interesting. Insights to the conformational flexibility of this drug might lead to a better understanding of the class of non-steroidal anti-inflammatory drugs that ibuprofen belongs to.
The spectrum was recorded with our broadband chirped-pulse Fourier transform microwave spectrometer in the frequency range of 2.0 - 8.3 GHz. With the obtained results, we are able to identify several conformers of ibuprofen and to determine their rotational constants. Density functional theory calculations were performed and used to support the conformational assignments. Fragments of ibuprofen could be also identified in the spectrum, which can be explained by thermal decomposition during the heating process for vaporizing it. The analysis of this fragmentation process as a function of temperature might provide us with some interesting insights into its mechanism.

[a]The author thanks "The Hamburg Centre for Ultrafast Imaging" for financial support.