THE CARBODIIMIDE SPECTRUM IN THE WAVENUMBER RANGE OF 450-1000 cm^{-1} AND IN THE THz REGION

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Carbodiimide, HNCNH, is an accidently nearly symmetric top molecule ($\kappa = -0.99999537$) and it undergoes internal rotation hindered by a *cis* and a *trans* energy barrier of nearly equal height of about 2070 cm^{-1}. This internal motion leads to torsional splittings of the rotational energy levels, which show an unusual dependence on the K_a rotational quantum number. The strong coupling between the torsional and the HNC bending motion leads to rotationally dependent contributions to the effective torsional potential function. To extend our knowledge about these complex internal motions and the structure of the molecule we recorded the spectrum of the equilibrium mixture of carbodiimide and cyanamide, H_2NCN, with a Bruker IFS 120HR in the range from 450 to 1000 cm^{-1}. Unfortunately the strong dominance of cyanamide (approximately 115:1 at 110°C) makes it very difficult to identify the torsional fundamental vibration. However, the antisymmetric HNC-bending fundamental could be analysed. To support the assignment procedure $ab-initio$ calculations using the CCSD(T) method had been carried out.
Spectra of the terahertz region offer the opportunity to study another remarkable property of the molecule, namely the recently observed inversion of the $K_a = 2$ energy levels[a] and the shift of the $K_a = 1$ levels due to a centrifugal distortion interaction with $\Delta K_a = 4$. We have now measured and analysed the ${}^rQ_1$ branch at 1.1 THz. The analysis of the terahertz data and the infrared data in the light of the recent ab-initio calculations will be presented.

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[a] V. Wagener, M. Winnewisser, M. Bellini, J. Mol. Spectrosc. 170, 323 (1995)