INFRARED STEPTROSCOPY ON CARBON CHAIN MOLECULES: REVISED MEASUREMENTS ON C_7

THOMAS F. GIESEN, PETRA NEUBAUER-GUENTHER, JÜRGEN KRIEG, STEPHAN SCHLEMMER,
I. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln.

The formation of pure carbon chain molecules, C_n (n=3, 4, 5, ...), plays an important role in interstellar chemistry and in combustion processes as well. Spectroscopic studies and high level *ab initio* calculations have been performed in recent years to derive molecular properties such as structure, vibrational dynamics, and electronic configuration of pure carbon clusters. Ro-vibrational transitions of asymmetric stretching modes lie in the mid-infrared region at 5 μm whereas transitions from energetically low lying bending modes are expected to occur in the Terahertz region. To date only the bending mode of C_3 has been directly measured by high resolution spectroscopy [1]. The search for bending mode transitions of longer carbon chain molecules is supported by recent large-scale coupled cluster calculations (see e.g. [2]) and by precise infrared measurements of asymmetric stretching modes and associated hot bands. Heath et al. used infrared laser absorption spectroscopy to measure the ν_4 fundamental and associated ν_{11} hot band of C_7 at 2137 cm^{-1} [3]. The authors found strong evidence for extremely large amplitude, anharmonic bending modes and concluded C_7 to be a fairly floppy molecule. This finding is in contradiction to recent high level *ab initio* calculations by Botschwina [4] who found no evidence of floppiness for the C_7 chain molecule, and therefore revised measurements are strongly needed.
In this paper we present high resolution tunable infrared diode laser measurements on the C_7 fundamental stretching mode ν_4 and associated hot band transitions $\nu_{11} - (\nu_4 + \nu_{11})$ at 2137 cm^{-1} to clarify the question of C_7 floppiness. Improved molecular constants for the fundamental band as well as for the hot band have been derived. We could not find any evidence for a large amplitude bending mode of C_7. All results are in very good agreement with calculations by Botschwina.

[1] C.A. Schmuttenmaer, R.C. Cohen, N. Pugliano et al., *Science* 249, 897 – 900 (1990).
[2] Botschwina *Theoretical Chemistry Accounts* 114, 350-356 (2005)
[3] J.R. Heath, R.J. Saykally, *J. Chem. Phys.* 94, 1724 (1991)
[4] P. Botschwina, *Chem. Phys. Lett.* 354, 148 (2002)