

## INFRARED SPECTROSCOPY ON CARBON CHAIN MOLECULES: REVISED MEASUREMENTS ON C<sub>7</sub>

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The formation of pure carbon chain molecules, C<sub>n</sub> (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<sub>3</sub> 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<sub>4</sub> fundamental and associated ν<sub>11</sub> hot band of C<sub>7</sub> at 2137 cm<sup>-1</sup> [3]. The authors found strong evidence for extremely large amplitude, anharmonic bending modes and concluded C<sub>7</sub> 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<sub>7</sub> chain molecule, and therefore revised measurements are strongly needed.

In this paper we present high resolution tunable infrared diode laser measurements on the C<sub>7</sub> fundamental stretching mode ν<sub>4</sub> and associated hot band transitions ν<sub>11</sub> - (ν<sub>4</sub> + ν<sub>11</sub>) at 2137 cm<sup>-1</sup> to clarify the question of C<sub>7</sub> 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<sub>7</sub>. 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)