Molecular structure of C_3 as determined by high-resolution spectroscopy

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Breier et al. [1] measured the lowest mode of C_3, ν_2 (63 cm^{-1}), using a teraherz supersonic-jet spectrometer in combination with a laser-ablation source. They recorded the spectra in the frequency range from 1.8 to 1.9 THz for normal and all ^{13}C-substiututed species, and reported precise spectroscopic constants for 12-12-12, 12-13-12, 13-12-13, 13-13-13, 13-12-12, and 13-13-12 isotopologues.

The C_3 radical was produced by by the laser ablation of a carbon target: the fourth harmonic of a Q-switched Nd:YAG laser at a 30 Hz repetition rate. The ablated carbon was seeded in a helium gas at 2 bar pressure which pre-expanded into a reaction channel of 3 mm length and 10 × 1 mm^2 cross section. The reaction channel allowed the formation of small and medium sized carbon clusters at moderate temperatures before the gas flow expanded adiabatically into a vacuum chamber in the form of a supersonic jet.

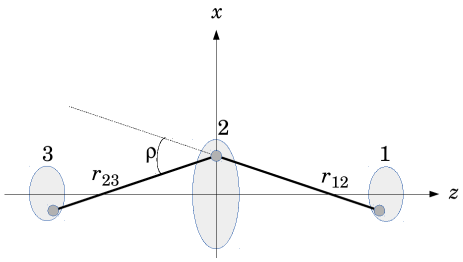

Fig. 1: Structure parameters

The radiation source was a synthesizer, from 9 to 14 GHz, whose out-put was amplified and frequency multiplied by a factor of 144 by a multiplier chain; generated radiation is from 1.8 to 1.9 THz. The THz-radiation crossed the supersonic jet perpendicularly 20 mm down-stream of the slit-nozzle in a Heriott-type multi-path optics. The transmitted THz-radiation was focused onto a liquid-He cooled InSb hot-electron bolometer.

The obtained spectra were analyzed by a standard Hamiltonian for linear molecules employing the PGOPHER program package [2]. The structure parameters, $r=r_{12}=r_{13}$ and ρ defined in Fig. 1, were evaluated for r_0-, r_s-, r_m- and r_e-structure. The nuclear distance r obtained for r_0-structure with the assumption of linear structure is anomalously shorter than the value of r_e predicted by an *ab initio* calculation [3].

This anomaly is caused by the large amplitude nature of the ν_2 mode. In the symposium the problems in the structure determination of the C_3 radical will be discussed in detail in comparison with a well-behaved linear molecule, CO_2 (Fig. 2).

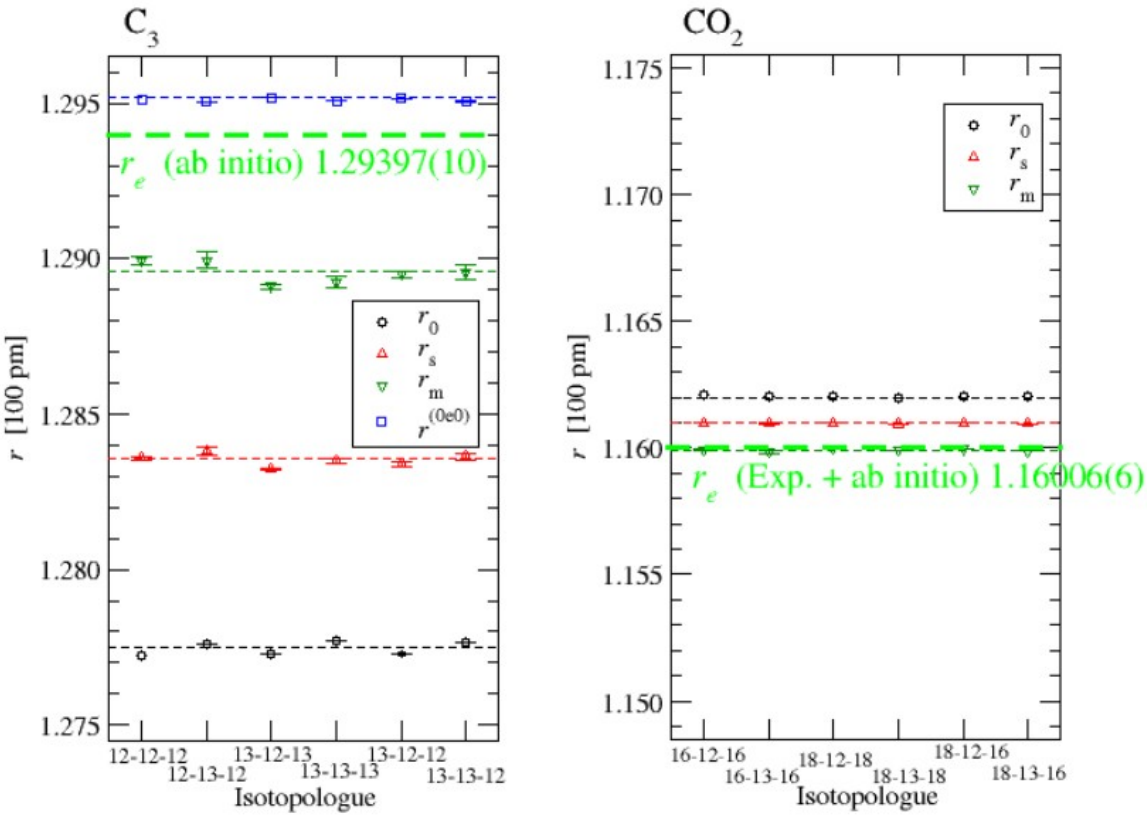

Fig. 2: Structure parameters of C_3 and CO_2

[1] A. A. Breier, T. Büchling, R. Schnierer, V. Lutter, G. W. Fuchs, K. M. T. Yamada, B. Mookerjea, J. Stutzki, and T. F. Giesen, *J. Chem. Phys.* **145**, 234302 (2016).

[2] C. M. Western, "PGOPHER: A program for simulating rotational, vibrational and electronic spectra," *J. Quant. Spectrosc. Radiat. Transfer,* **186**, 221 (2017).

[3] B. Schröder and P. Sebald, *J. Chem. Phys.* **143**, 224312 (2015).