

## STRETCHING OUR KNOWLEDGE OF THE ELECTRONIC GROUND STATE OF C<sub>3</sub>: THE SPECTROSCOPY OF STRETCHING MODES OF C<sub>3</sub>

KIRSTIN D DONEY<sup>a</sup>, *JILA and NIST, University of Colorado, Boulder, CO, USA*; BENJAMIN SCHRÖDER, *Institute of Physical Chemistry, Georg-August-Universität Göttingen, Göttingen, Germany*; DONGFENG ZHAO, *Hefei National Laboratory for Physical Science at Microscale, University of Science and Technology of China, Hefei, China*; PETER SEBALD, *Institute of Physical Chemistry, Georg-August-Universität Göttingen, Göttingen, Germany*; HAROLD LINNARTZ, *Leiden Observatory, Sackler Laboratory for Astrophysics, Universiteit Leiden, Leiden, Netherlands*.

We present the high-resolution spectrum of C<sub>3</sub> produced in a supersonically expanding propyne plasma, which is recorded around 3 μm using continuous wave cavity ring-down spectroscopy (cw-CRDS). Fifteen fully resolved ro-vibrational bands are observed, which have been assigned to vibrationally excited  $n\nu_1+m\nu_3$  combination bands of C<sub>3</sub>; fourteen of which are reported for the first time. This work is a significant extension of the known electronic ground state vibrational energy levels, with the observed number of quanta being:  $n \leq 7$  and  $m \leq 3$ . Furthermore, with the new observations of highly excited vibrational modes, up to the (7,0,1) energy level, we are able to test the fundamental understanding of this "floppy" benchmark molecule. A detailed analysis of the experimental spectra is supported by ro-vibrational calculations based on an accurate local *ab initio* potential energy surface (PES) for C<sub>3</sub> ( $\tilde{X}^1\Sigma_g^+$ ).<sup>b</sup> The presented variational calculations give remarkable agreement compared to experimental values with typical accuracies of ~0.01% for the vibrational frequencies and ~0.001% for the rotational parameters, even for high energy levels around 10000 cm<sup>-1</sup>.<sup>c</sup>

<sup>a</sup>Previously at Universiteit Leiden (Sackler Laboratory for Astrophysics).

<sup>b</sup>B. Schröder and P. Sebal, *J. Chem. Phys.* 144, 044307 (2016)

<sup>c</sup>B. Schröder *et al.*, *J. Chem. Phys.* 149, 014302 (2018)