

STRETCHING OUR KNOWLEDGE OF THE ELECTRONIC GROUND STATE OF C₃: THE SPECTROSCOPY OF STRETCHING MODES OF C₃

KIRSTIN D DONEY^a, *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 C₃ 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 C₃; 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 C₃ ($\tilde{X}^1\Sigma_g^+$).^b 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⁻¹.^c

^aPreviously at Universiteit Leiden (Sackler Laboratory for Astrophysics).

^bB. Schröder and P. Sebald, *J. Chem. Phys.* 144, 044307 (2016)

^cB. Schröder *et al.*, *J. Chem. Phys.* 149, 014302 (2018)