HIGH RESOLUTION OVERTONE SPECTROSCOPY OF THE ACETYLENE VAN DER WAALS DIMER, $^{12}(C_2H_2)_2$

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CW-cavity ring down spectroscopy was used to record in a free jet expansion the spectrum of the absorption band in $(^{12}C_2H_2)_2$ with origin at 6547.6 cm^{-1}. It is a perpendicular band and corresponds to 2CH excitation in the hat unit of the T-shaped dimer. Calibration (better than $\pm 1 \times 10^{-3}$ cm^{-1} accuracy) and ring-down time (130 μs) were improved compared to a previous contribution [a], and a line-by-line analysis was undertaken. Three series of lines were identified involving levels with A1$^+$, E$^+$ and B1$^+$ tunneling symmetries, confirming the spectral and symmetry analyses reported in the literature for the 1CH excitation band [b]. 164 vibration-rotation-tunneling lines were assigned in the $K'_a - K''_a = 2-3, 0-1, 2-1$ and $4-3$ sub-bands and effective rigid rotor vibration-rotation constants were obtained by simultaneously fitting 1CH and 2CH lines from the same symmetry series. Perturbations affecting the K_a stacks, in particular, are reported. The tunneling frequency in 2CH is estimated to be $\nu^{2CH}_{tunn.}$ = 270 MHz for the K_a = 0 stack. The rotational temperature is determined to be 23 K from relative line intensities and the half lifetime of the dimer in the 2CH hat state is estimated to 1 ns from individual line widths.

[a] Didriche *et al.*, *Mol. Phys.* 2010, **108**, 2158-2164
[b] Fraser *et al.*, *J. Chem. Phys.* 1988, **89**, 6028-6045