ROTATIONAL SPECTRA OF THE CH_3CN-CO_2 COMPLEX: OBSERVING A CARBON 'TETREL BOND'

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The CH_3CN-CO_2 complex was investigated using a pulsed nozzle Fourier transform microwave spectrometer. Nitrogen containing compounds generally form a T-shaped complex with CO_2 having a N-CO_2 'tetrel bond'. For example, microwave spectrum confirmed this structure for HCN-CO_2 back in 1984, though specific names of intermolecular bonds were not used those days[a]. We have observed two structures for the CH_3CN-CO_2 complex, the T-shaped and a π-stacked (the CO_2 is parallel to the CH_3CN). The ab initio calculations show that the two structures have similar binding energies. The T-shaped structure has a nearly prolate 'a'–type spectra with the K=1 lines missing, which is consistent with the C_{2v} symmetry of the T-shaped structure. All rotational transitions observed show hyperfine splitting due to nuclear quadrupole coupling of the nitrogen atom. Measurements with isotopic substitutions have been carried out to ascertain the assignment of the rotational transitions.

[a]Leopold, K. R.; Fraser, G. T.; Klemperer, W. J. Chem. Phys. 1984, 80, 1039–1046.