ROTATIONAL SPECTROSCOPIC STUDIES ON THE CH_3CN-CO_2 COMPLEX

SHARON PRIYA GNANASEKAR, ELANGANNAN ARUNAN, *Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore, India.*

The CH_3CN-CO_2 complex was investigated using a Pulsed-Nozzle Fourier Transform Microwave Spectrometer. This complex offers the possibility of observing a 'carbon-bonded' structure. The ab initio calculations give three minima structures; a π-stacked structure, a T-shaped structure with the N end of CH_3CN interacting with the C atom of CO_2, and a linear structure with the O of CO_2 interacting with the tetrahedral C of CH_3CN. Thus, the T-shaped and the linear structures are bound with a 'carbon-bond'. The π-stacked and T-shaped structures have similar binding energies (-7.7 kJmol^{-1} and -7.6 kJmol^{-1}, respectively). Many lines were observed which depend on both CH_3CN and CO_2 concentrations. Six of these lines follow a nearly prolate, 'a'-type spectra. The K=0 (J = 3-2 to 8-7) rotational transitions have been observed. The B+C value obtained from fitting these transitions is consistent with the value predicted for the T-shaped geometry with an N-C interaction. All lines show hyperfine splitting due to quadrupole coupling of the nitrogen atom. Measurements with isotopic substitutions have been carried out to ascertain the assignment of the rotational transitions. The unassigned lines may belong to the other possible geometries of the CH_3CN-CO_2 complex.