ROTATIONAL SPECTROSCOPY OF THE PYRIMIDINE-CO_2 COMPLEX

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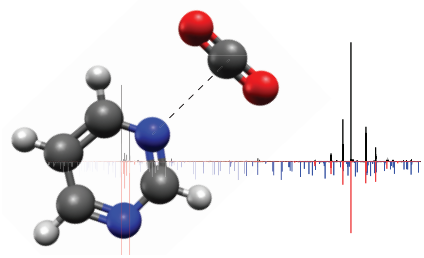

The looming threat of anthropogenic climate change has driven a significant amount of research into efficient methods of capturing and storing[1] CO_2. Reversible capture mechanisms, such as those governed by weakly bound intermolecular interactions, have been a mainstay of such research.

To this end, the rotational spectrum of the pyrimidine ($C_4H_4N_2$)-CO_2 van der Waal's complex has been measured using broadband chirped-pulse Fourier transform microwave (CP-FTMW) spectroscopy across a frequency range of 7.5 to 17.5 GHz, in an effort to investigate the viability of pyrimidine as an active site in CO_2 capture media.

A preliminary fit of the spectrum indicates a structure whereby the lone pair of one of the nitrogen atoms is directed towards the CO_2 carbon atom, with the O=C=O axis lying in the plane of the pyrimidine moiety and approximately perpendicular to a line drawn through the corresponding nitrogen atom and the pyrimidine centre-of-mass. This is analogous to the structure of the pyridine-CO_2 complex[2], and in agreement with the structures predicted by DFT calculations performed at a wB97XD/6-311++G** level of theory, as well as previously published computational studies[3]. The principal rotational constants produced by this fit are: A = 4070.9905(46) MHz, B = 859.4088(12) MHz and C = 710.01942(85) MHz.

[1] C. Yu, *et. al.*, *Aerosol Air Qual. Res.* **2012**, *12*, 745-769
[2] J. L. Doran., *et. al.*, *J. Mol. Struct.* **2012**, *1019*, 191-195
[3] K. D. Vogiatzis, *et. al.*, *ChemPhysChem* **2009**, *10*, 374-383