INVESTIGATION OF THE AMIDE I BAND OF N-METHYLACETAMIDE IN SOLID PARAHYDROGEN USING FTIR SPECTROSCOPY

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We report the FTIR spectra of the Amide I and Amide A vibrational modes of N-methylacetamide (NMA, $CH_3CONHCH_3$) isolated in a solid parahydrogen (pH_2) matrix. NMA is one of the simplest molecules that contains the peptide bond and has therefore been the subject of numerous studies, especially those concerning peptide structure and dynamics. Solid pH_2 is a unique quantum solid matrix host that, among other features, allows for high-resolution IR studies of trapped dopant species. In our preliminary report,[a] we showed that the Amide I lineshape was surprisingly broad and shifts were observed with small changes in temperature. That talk did not resolve the origin of these shifts with temperature that require many minutes to fully equilibrate. Further investigations have revealed that the frequency and breadth of the transition depends partially on the orthohydrogen concentration in the matrix. The Amide I lineshape displays both reversible and irreversible components that are dependent upon the temperature of the host matrix. This talk will discuss possible explanations for the breadth and temperature dependence of the Amide I feature of NMA isolated in solid pH_2.

[a] L. O. Paulson and D. T. Anderson, *61st Ohio State University International Symposium on Molecular Spectroscopy,* talk R008 (2006)