EXPLORING THE n→π* INTERACTION BETWEEN PYRIDINE AND KETONES: THE ROTATIONAL SPECTRUM OF PYRIDINE-ACETONE ADDUCT.

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The pyridine–acetone adduct generated in a supersonic expansion has been observed using chirped pulse Fourier transform microwave spectroscopy. The spectrum shows the characteristic multiplet structure due to the presence of the two equivalent methyl tops of acetone. The experimental structure shows the fingerprints of an n→π* interaction between the pyridine N atom lone pair and the acetone carbonyl group. This interaction is usually associated with the Bürgi-Dunitz trajectory of nucleophilic addition to a carbonyl compound. The observed methyl group internal rotation barrier is lower than that for free acetone. The structure and internal dynamics of the complex are compared to those of related adducts as pyridine-formaldehyde[a] and pyridine-acetaldehyde.[b] These complexes are an excellent benchmark for experiment and theoretical computations to explore the n→π* Bürgi-Dunitz coordinate and its interplay with the methyl group internal rotation.

[a] S. Blanco and J. C. López, *J. Phys. Chem. Letters* **2018**, *9*, 4632-4637

[b] S. Blanco, A. Macario and J. C. López, *Phys. Chem.Chem. Phys* **2019**, *21*, 20566-20570