P5493:
ROTATIONAL SPECTRUM OF 2-AMINOACETOPHENONE AND ITS 1:1 WATER COMPLEX

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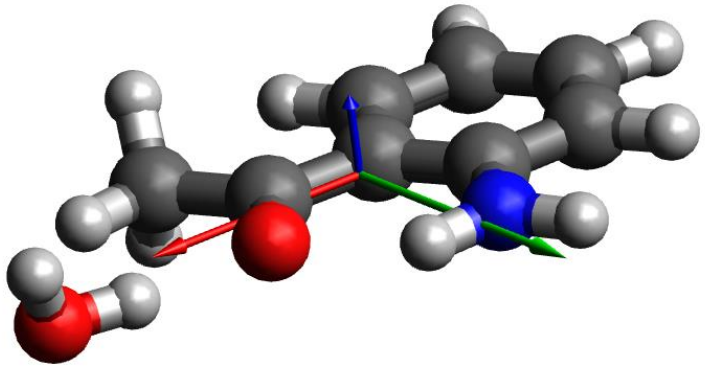
complex



No μ_c-type transitions
M_{cc} 2.2 (uÅ^2)
all monosubstituted ^{13}C
isotopologues at natural abundance

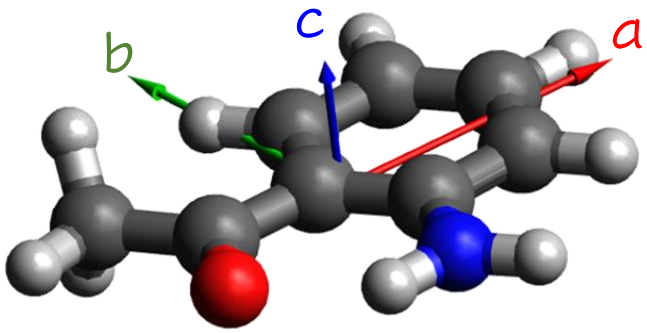
Methods

- Chirped Pulse - Fourier Transform microwave spectroscopy (2-8 GHZ)
- DFT method -> B3LYP/def2-TZVP

Main results

- Cs symmetry both for monomer and complex
- intramolecular HB responsible for the planarity of amino group differently from what observed for aniline

monomer



No μ_c-type transitions
M_{cc} 1.8 (uÅ^2)
all monosubstituted ^{13}C and ^{15}N
isotopologues at natural abundance