Supplementary Material (ESI) for Photochemical & Photobiological Sciences

Picosecond Time-Resolved Infrared Study of 2-Aminopurine Ionisation in Solution

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The DFT calculations for 7-H tautomer using Onsager model produce IR spectra significantly different from the gas phase and Langevin models. This is due to the change in the optimised geometry of 2AP. For 7-H tautomer within Onsager model the solvent forces 2AP to adopt a puckered conformation, while in all the other cases 2AP molecule remains flat.

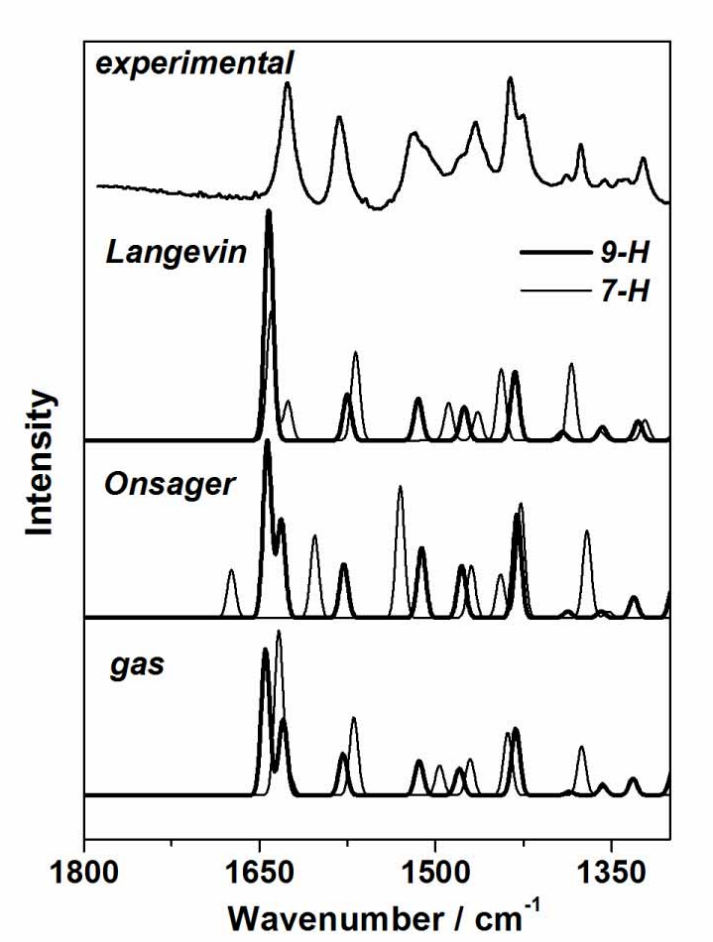

Figure 1 Experimental FTIR spectrum of 2-aminopurine (2AP) in D_2O solution at pD = 7 and IR spectra calculated for 7-H and 9-H tautomers of 2AP in the gas phase and in solution phase according to Onsager and Langevin models.

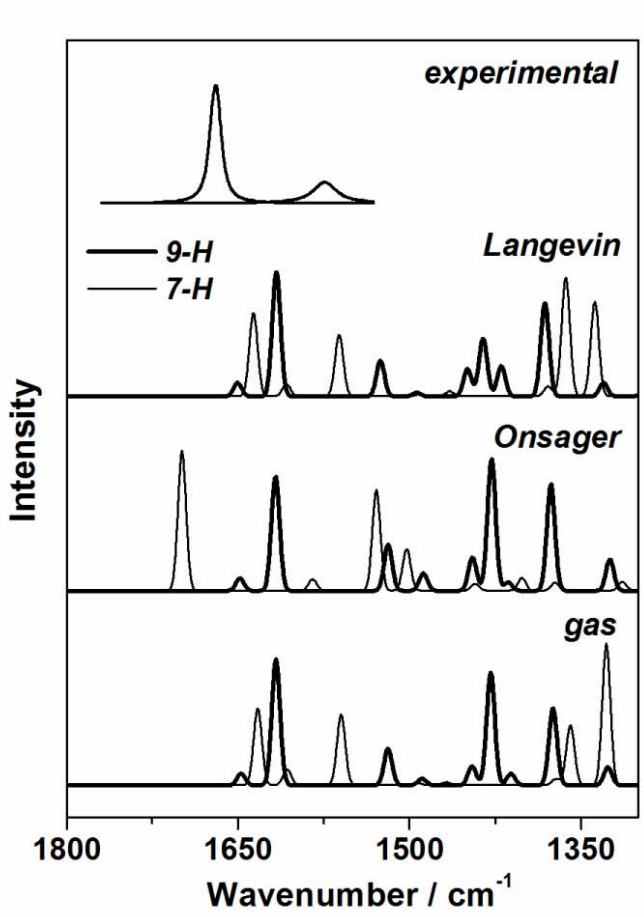

Figure 2 Transient bands observed in ps-TRIR experiment following 267 nm excitation of 2-aminopurine (2AP) in D_2O solution at pD = 2 and IR spectra calculated for 7-H and 9-H tautomers of 2-aminopurine radical cation, $2AP^{+\bullet}$, calculated in the gas phase and in solution phase according to Onsager and Langevin models.

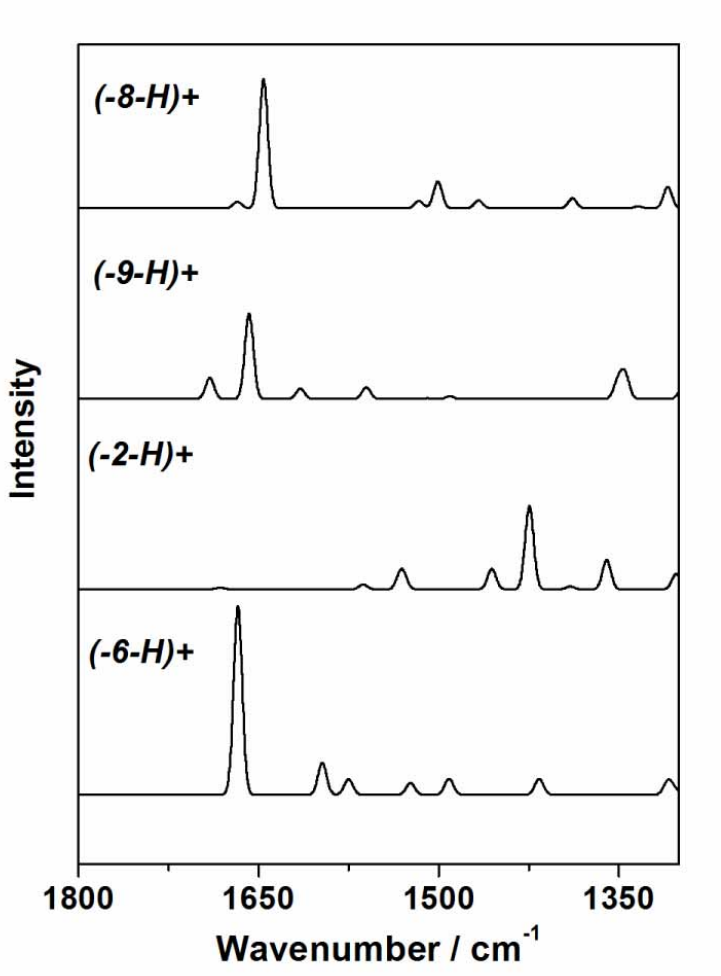

Figure 3 IR spectra calculated using Langevin model for 2-aminopurine neutral radical, $2AP^{\bullet}(-H^{+})$, deprotonated from different sites.