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Solvent effects on the π^* shape resonances of uracil

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ABSTRACT

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resonances of uracil, referred to as π_1^* and π_2^* in the order of increasing energy. Our study considered uracil–water aggregates with six solvent molecules obtained from Monte Carlo simulations in the liquid phase. To explore the ensemble statistics, we combined scattering calculations, performed in the static exchange and static exchange plus polarization approximations, with linear regressions of virtual orbital energies to the scattering results. In general, the solvent molecules stabilize the anion states, and the lower lying π_1^* resonance becomes a bound state in most of the solute–water clusters. We also discuss how the strength of the H bonds can affect the energies of the anion states, in addition to the number and donor/acceptor characters of those bonds. The thermal distributions for the vertical attachment energies, obtained from 133 statistically uncorrelated solute–solvent clusters, are significantly broad in the energy scale of the autoionization widths. The distributions for the π_1^* and π_2^* anion states slightly overlap, thus giving rise to a quasi-continuum of attachment energies below $\lesssim$2.5 eV, in contrast to the gas phase picture of electron attachment to well separated resonances below the electronic excitation threshold. Both the stabilization of the anion states and the spread of attachment energies could be expected to favor the dissociative electron attachment processes believed to underlie the electron-induced damage to biomolecules.

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