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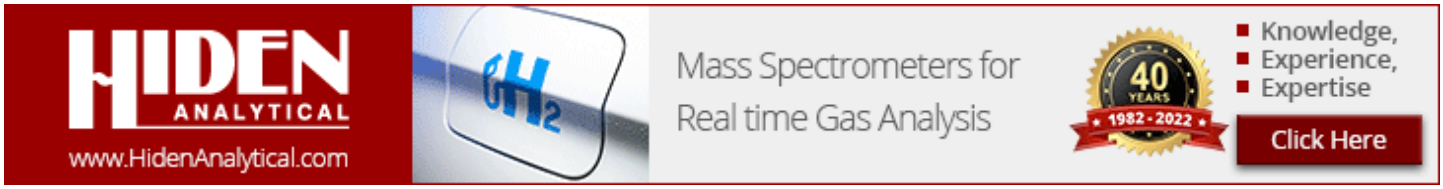

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Shape resonance spectra of uracil, 5-fluorouracil, and 5-chlorouracil

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We report on the shape resonance spectra of uracil, 5-fluorouracil, and 5-chlorouracil, as obtained from fixed-nuclei elastic scattering calculations performed with the Schwinger multichannel method with pseudopotentials. Our results are in good agreement with the available electron transmission spectroscopy data, and support the existence of three π* resonances in uracil and 5-fluorouracil. As expected, the anion states are more stable in the substituted molecules than in uracil. Since the stabilization is stronger in 5-chlorouracil, the lowest π* resonance in this system becomes a bound anion state. The present results also support the existence of a low-lying σ^*_{CCl} shape resonance in 5-chlorouracil. Exploratory calculations performed at selected C–Cl bond lengths suggest that the σ^*_{CCl} resonance could couple to the two lowest π* states, giving rise to a very rich dissociation dynamics. These facts would be compatible with the complex branching of the dissociative electron attachment cross sections, even though we cannot discuss any details of the vibration dynamics based only on the present fixed-nuclei results.

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