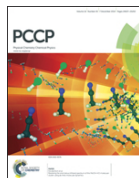


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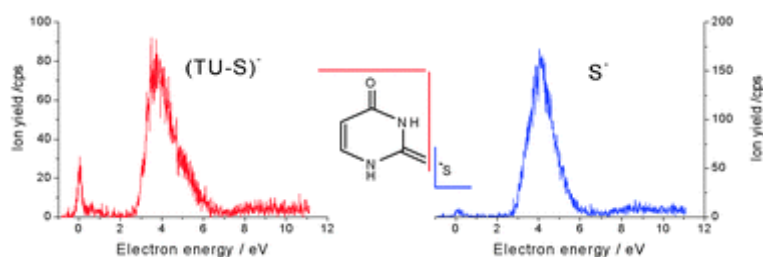
Physical Chemistry Chemical Physics

Electron driven reactions in sulphur containing analogues of uracil: the case of 2-thiouracil

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Abstract

The fragmentation of 2-thiouracil (TU) molecules induced by low energy (<12 eV) electrons is investigated experimentally and theoretically. It is observed that most of the damage is localised at the sulphur site and in particular visible *via* the production of the thiocyanate, SCN^- , anion. Similar to the canonical nucleobases the loss of the hydrogen atom is a predominant dissociation channel already at the subexcitation energies. The theory shows that for incident electron energies below 3 eV dissociative electron attachment is initiated by shape resonances implicating the π^* molecular orbitals. It may also arise from the dipole bound supported state as illustrated by the production of the SCN^- , S^- and $(\text{TU-S})^-$ fragments observed close to 0 eV but also the formation of $(\text{TU-H})^-$ species at 0.7 and 1 eV.



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