Low-energy electron interactions with 5-Nitro-2,4-Dichloropyrimidine: Anion States and Likely Dissociation Pathways

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We report a computational study of the anion states of the 5-Nitro-2,4-Dichloropyrimidine (NDP) molecule employing both bound state and scattering techniques [1], also investigating dissociative electron attachment (DEA) pathways. Although the NDP molecule proved to be toxic, it was recently pointed out [2] as a universal model for elementary processes induced by electrons underlying the radiosensitizing action. The compound presents a unique combination of the mechanisms usually credited for the action of radiosensitizers, pointing to a new paradigm, in which drugs may have several mechanisms underlying their biological activity. Our calculations indicate two valence bound states (π_1* and π_2*) and three resonances (σ_{CCl1}*, σ_{CCl2}* and π_4*) for that system. The computed thermodynamic thresholds are compatible with DEA reactions producing $[NDP\text{-}NO]^-$ and $[NDP\text{-}NO_2]^-$ at 0eV [2] indicating that the anion bounded states are expected to account for these eliminations, probably involving a π*/σ* couplings along the vibration dynamics. At higher energies, our results indicate that dissociation occurs via a direct DEA mechanism for more intense fragments.

References

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