

Abstract Submitted
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Calculation of Positron Binding Energies and Implications for Feshbach-Resonant Positron-Uracil Annihilation INDIKA WANNIARACHCHI, CAROLINE MORGAN — Here we investigate by first-principles calculations the possible role of vibrational Feshbach resonances in enhancing positron annihilation for low-energy positron beams incident on uracil, a base found in RNA. Geometries, vibrational polarizabilities, and dipole moments for uracil and 5-halouracils are calculated with density functional theory, DFT-B3LYP with a 6-31G+(d, p) basis set, and are used to determine positron-uracil and positron-5-halouracil binding energies. The energy of the Feshbach resonances is then determined by the law of energy conservation. Experimental work on positron interactions with uracil and 5-halouracils in conjunction with the theoretical work reported here is underway.

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