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Low-energy electron scattering from the aza-derivatives of pyrrole, furan, and thiophene

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F. Kossoski¹ and M. H. F. Bettega^{2, a)}

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ABSTRACT

We report elastic integral and differential cross sections for electron scattering from the aza-derivatives of pyrrole, furan, and thiophene, namely, pyrazole, imidazole, isoxazole, oxazole, isothiazole, and thiazole. The calculations were performed within the Schwinger multichannel method with pseudopotentials, with inclusion of static, exchange, and polarization interactions, for energies up to 10 eV. We found two π^* shape resonances and a high-lying σ^* shape resonance in each system. A sharp low-energy σ^* resonance was also identified in isothiazole and thiazole. Pyrazole and imidazole presented yet a broad low-lying σ^* resonance. The positions of the resonances agree very well with existing experimental results. We discuss the similarities and differences among the resonances of these compounds.

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