VALIDATING WAVEFUNCTIONS IN MOMENTUM SPACE: A COMPUTATIONAL AND EXPERIMENTAL ELECTRON MOMENTUM SPECTROSCOPIC STUDY OF 2,6-STELLADIONE

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The ground electronic state for 2,6-stelladione ($C_8H_8O_2$, X^1A_1), has been studied using quantum mechanical calculations such as density functional theory (DFT) calculations. Based on these calculations and the plane wave impluse approximation (PWIA), the momentum distributions (MDs) of a set of representable outer valence MOs for the 2,6-stelladione have been simulated. The simulated MDs are compared against our first time measurements using high-resolution electron momentum spectroscopy (HREMS). Such a detailed comparison between the experimental MDs and simulated MDs provides insight and understanding of the electron correlation effects as well as the orbital relaxation effects on the MOs. In addition, the accuracy of the DFT exchange-correlation (XC) functionals used and the basis sets tested.