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An Electron Momentum Spectroscopy, Density Functional and Greens Function Theories study of the Outer Valence Electronic Structure of Bicyclo[2.2.1]heptane-2,5-dione MICHAEL BRUNGER, DARRYL JONES, School of Chemistry, Physics and Earth Sciences, Flinders University, STEFAN KNIPPENBERG, JEAN-PIERRE FRANCOIS, MICHAEL DELEUZE, Department SBG, Limburgs Universitair Centrum, SAUMITRA SAHA, FENG WANG, Centre for Molecular Simulation and School of Information Technology, Swinburne University of Technology, ROLF GLEITER, JOHANNES BUEBER, Organic Chemistry Institute, University of Heidelberg, DAVE WINKLER, CSIRO Molecular Science — We report our preliminary results for an electron momentum spectroscopy (EMS) study of the outer valence electronic region of bicyclo[2.2.1]heptane-2,5-dione. The measured binding energy spectra are presented for the azimuthal angles 0°, 10° and 0°+10° and are compared to new He(Iα) photoelectron spectroscopy results. These data are then compared with results from theoretical computations, using Greens Function theories. Derived momentum distributions are compared against those obtained by calculations which employ the plane-wave impulse approximation. These calculations use basis sets obtained from Density Functional Theory calculations at the triple zeta valence polarization level with a collection of different exchange correlation functionals.

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