Abstract Submitted
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Electron-Impact Ionization of Biomolecules.[1] ESAM ALI, Northwest Missouri State University, Maryville, Missouri, USA, DON MADISON, Missouri University of Science Technology, HIMADRI CHAKRABORTY, Northwest Missouri State University, Maryville, Missouri, USA — We report theoretical molecular 3-body distorted wave (M3DW) fully differential cross sections for electron impact ionization of several DNA analogue molecules. These results are useful to model the role of electrons in causing damage to DNA in biological systems [1]. Since experimental measurements do not determine the orientation of the molecule at the time of ionization, theoretical calculations must average over all possible orientations. Owing to computational limitations, our earlier work introduced the orientation averaged molecular orbital (OAMO) approximation, but the overall agreement with experiment was not very good [2]. While OAMO seemed to work better for larger molecules, it did not predict the detailed structures seen in the data. Our current treatment, however, improves the method where the cross section is calculated for a number of different molecular orientations and then numerically averaged. This proper averaging technique yields much better agreement with experiment [3]. We will show results and comparisons for several DNA analogue molecules in the conference. [1] Sanz *et al.*, *Int. J. Radiat. Biol.* **88**, 71 (2012); [2] Gao *et al.*, *J. Chem. Phys.* **123**, 204302 (2005); [3] Esam Ali, H. S. Chakraborty, and D. H. Madison (submitted).

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