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Accuracy of OAMO (Orientation Averaged Molecular Orbital) approximation for calculating electron-impact ionization cross sections for molecules[1] ADAM UPSHAW, BEN PAYNE, Missouri S&T, JAMES COLGAN, Los ALamos National Lab., DON MADISON, Missouri S&T — We have been using the M3DW (molecular 3-body distorted wave) approximation plus the OAMO (orientation averaged molecular orbital) to calculate cross sections for electron-impact ionization of molecules. The approximation yielded good agreement with experiment for H2 and reasonable agreement for N2. However, the agreement was not that good for H2O, CH4, and larger molecules so the important question concerns if the disagreement is a result of the OAMO approximation or a problem with the theoretical approach. Consequently we have modified our computer codes to perform a proper average over molecular orientations. M3DW results both with and without making the OAMO approximation will be compared with experimental measurements.

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