Abstract Submitted
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Calculating electron-impact ionization cross sections for molecules without making orientation averaging approximation[1] ADAM UPSHAW, DON MADISON, Missouri S and 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 H_2 and reasonable agreement for N_2. However, the agreement was not that good for H_2O, CH_4, and larger molecules and at least part of the problem must be attributed to the OAMO approximation. Consequently, we have dropped the OAMO approximation and have performed a proper numerical average over al orientations. M3DW results both with and without making the OAMO approximation will be compared with experimental measurements.

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