Abstract Submitted
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A Simple Method to Calculate Elastic Scattering of Electrons by Molecules of any Size[1] MIKE CRABTREE, DON MADISON, University of Missouri-Rolla — We have developed a simple method to calculate differential cross sections for elastic scattering of electrons from molecules. The computer program called General Atomic and Molecular Structure System, or GAMESS, is used to generate molecular charge densities. The charge densities are used to calculate spherically averaged static potentials for an external electron. To the static potential, we add approximate correlation, polarization and exchange potentials. The resulting molecular potential is then used to calculate L- dependent phase shifts and elastic scattering cross sections. The accuracy of this simple method will be examined by comparing theoretical results with absolute differential cross section measurements that have been made for several different molecules.

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