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Static potentials for electron-molecule scattering: the case of water ALLAN STAUFFER, Department of Physics and Astronomy, York University, Toronto, Canada, TAPASI DAS, RAJESH SRIVASTAVA, Department of Phyics, Indian Institute of Technology, Roorkee, India — Molecular wave functions are commonly represented by Gaussian orbitals which have a simple form. We have derived a scheme to calculate spherically-averaged static potentials for electron-molecule scattering which is analytic except for the inclusion of the error function which can be easily calculated using existing algorithms. Although the asymptotic form of these potentials falls off too rapidly, the scattering potential is dominated by the long range polarization potential in this region. Including an exchange potential produces a result which is realistic representation of the electron-molecule interaction. Details of the method will be presented as well as an application to electron scattering from water. Our method produces results in good agreement with existing calculations and experimental measurements. The extension of this method to more complex molecules is straightforward.

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