AB INITIO STUDY OF LOW-ENERGY ELECTRON COLLISIONS WITH ETHYLENE

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We present the results of an investigation of elastic electron scattering by ethylene, C_2H_4, with incident electron energies ranging from 0.5 to 20 eV, using the complex Kohn variational method. These are the first fully *ab initio* calculations to accurately reproduce experimental angular differential cross sections at energies below 3 eV. Low-energy electron scattering by ethylene is sensitive to the inclusion of electronic correlation and target-distortion effects. We therefore report results that describe the dynamic polarization of the target by the incident electron and involve calculations over a range of different geometries, including the effects of nuclear motion in the resonant $^2B_{2g}$ symmetry with an adiabatic nuclei treatment of the C-C stretch mode. The inclusion of dynamic polarization and the effect of nuclear motion are equally critical in obtaining accurate results. The calculated cross sections are compared with recent experimental measurements.

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I. INTRODUCTION

Collisions of electrons with small polyatomic molecules are important in many areas of physics. They are of interest in determining the energy balance and transport properties of electrons in low-temperature gases and plasmas under a wide variety of conditions. Electron-molecule collision data is critically important for numerical modeling studies [1] in wide-ranging areas such as plasma deposition and etching of semiconductors, gaseous high voltage switches and environmental remediation plasmas.

Electron scattering by hydrocarbons is particularly relevant to cold plasma technology. Although ethylene, C_2H_4, is one of the simpler hydrocarbon molecules, there have been only very limited studies of its interaction with low-energy electrons.

Low-energy electron scattering by atoms and molecules can be dominated by electrostatic interaction effects, electron exchange, and electron correlation. The proper balance of these effects is needed to theoretically describe effects such as the Ramsauer-Townsend (RT) effect. Shape resonances are also sensitive to the effects of electron correlation and, in addition, are sensitive to changes in target nuclear geometry. The proper inclusion of all these factors is crucial for an adequate description of resonance parameters and vibrational excitation cross sections.

We present the results of an investigation of the collision of low-energy electrons with ethylene using the complex Kohn variational method. Ethylene is a closed-shell molecule which possesses a permanent quadrupole moment. Early *ab initio* calculations by Schneider *et al.* [2] were the first to confirm the existence of the Ramsauer-Townsend effect in such a molecule. Ethylene also has a low-lying shape resonance whose position and width are strongly influenced by target-distortion effects. The resonance is of $^2B_{2g}$ symmetry and corresponds to the temporary capture of the incident electron into an empty, antibonding, valence orbital. The investigations of Schneider *et al.* , which were carried out only at the equilibrium geometry and included only two scattering symmetries, produced a resonance at 1.83 eV, in excellent agreement with experiment. Several other theoretical studies on low-energy electron scattering from ethylene have been performed in the fixed-nuclei approximation at equilibrium geometry[3–5]. None of the previous calculations, however, have been particularly successful in describing experimental angular differential cross sections at electron impact energies below 3 eV, as evidenced by the recent experimental measurements of Panajotovic *et al.* [6].

The present calculations extend the work of Schneider *et al.* [2] by including all relevant symmetries and important dynamical correlation effects. In addition, the calculations include the effects of nuclear motion for the critically important resonant symmetry. It will be shown below that all these factors are essential in obtaining accurate total, momentum transfer, and elastic differential cross sections.

II. THEORETICAL FORMULATION

The complex Kohn method is a variational technique which uses a trial wave function that is expanded in terms of square-integrable (Cartesian Gaussian) and continuum basis functions that incorporate the correct asymptotic boundary conditions. Detailed descriptions of the method have been given in previous publications (see, for instance, refs. [7, 8]), so only a brief summary of the aspects that concern this study will be given below.

In the case of electronically elastic scattering, the trial wave function to be used is of the form: