Theoretical study of electron collision by OCS molecule: elastic process

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The electron collision with a carbonyl sulfide (OCS) molecule is one of the interesting processes in the earth's atmosphere, since the OCS molecule is a serious atmospheric pollutant. In the present work, a theoretical study is attempted to get detailed information about elastic scattering (more strictly, vibrationally elastic scattering, corresponding to the experimental data available) of electrons from OCS.

The present calculation method is basically the same as the case of elastic scattering of an electron from a carbon dioxide molecule[1] except in some respects. Hence, only some aspects of the theory are briefly mentioned here. We employ the *fixed-nuclei, adiabatic-rotation approximation*, that is, we freeze the target nuclei throughout the collision. In the incident energy region 1.0–60.0 eV, where the calculation is made, the electronic excitation probability of the target molecule is expected to be smaller than the elastic scattering probability. Therefore, the target molecule is assumed to stay in the electronically ground state, in which the OCS molecule is linear. The origin of the coordinates is located at the center-of-mass of the molecule and the body-fixed frame is employed, i.e., the z-axis is chosen along the molecular axis and the target nuclei are placed at the positions O(0, 0, -3.17817), C(0, 0, -0.99147), and S(0, 0, 1.95753). The wave function of the incident electron is expanded in terms of the spherical harmonics to yield coupled differential equations for the radial part of the wave function. We solve the coupled differential equations with the scattering boundary conditions to evaluate the scattering matrix (S-matrix) in the body-fixed frame. After the frame transformation from the body-fixed to the space-fixed coordinates, differential cross sections are obtained. To consider the effect of the long-range dipole interaction, the closure method (with the adiabatic-rotation version of the point-dipole-Born approximation) is adopted. The effect is significant in the forward scattering region.

The present electron-molecule interaction potential is composed of three terms: static, exchange and correlation-polarization potentials. For electron exchange, we use a local model potential, i.e., the Hara version of the free-electron-gas exchange model[2]. To take account of the target polarization, use is made of a parameter-free correlation-polarization model[3]. This model is constructed by matching local, short-range correlation potential to the long-range polarization potential. The former is evaluated in the local density approximation of electron gas. We use the quantum chemistry molecular orbital code *GAMESS* to generate the multi-centered target wave function.

Figure 1 compares the present differential cross section (DCS) for elastic scattering at

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an incident energy of 10.0 eV with the experimental DCS[4] and the theoretical values obtained by the continuum-multiple-scattering method[5] and by the Schwinger multichannel method[6]. The present calculation reproduces the experimental DCS fairly well and is also in a good qualitative agreement with the other theoretical results except at a scattering angle of 0°. The disagreement at 0° is due to the use of the closure relation with the "adiabatic" dipole-Born approximation, which leads to divergence at 0°. A calculation with consideration of the rotational transition should be needed to evaluate the appropreate DCSs in the forward scattering region[7].

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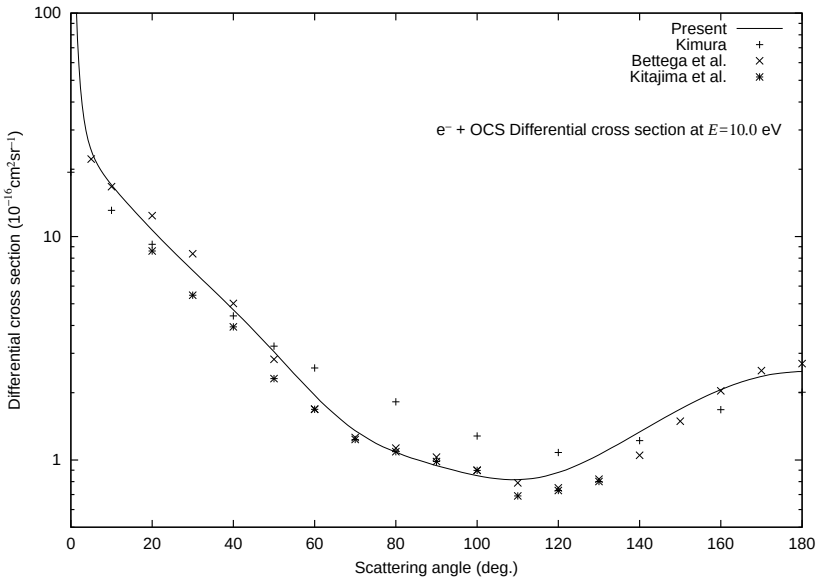

Figure 1: Differential cross sections for the elastic scattering at 10.0 eV.