

I-M Electron, Positron and Heavy Particle Scattering Dynamics

We are concerned with theoretical aspects on scattering dynamics resulting from electron, positron, and ion and atom collisions with polyatomic molecules. A few subjects we put emphasize are: (i) a comparative study of electron and positron scattering from polyatomic molecules, (ii) dissociative positron attachment, (iii) resonances in electron, positron and ion impacts on molecules, and (iv) atomic collisions at ultra-low temperature.

I-M-1 Strong Mode Dependence of 3.8-eV Resonance in CO₂ Vibrational Excitation by Electron Impact

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Vibrational excitation modes are significantly enhanced by the presence of the shape resonance at 3.8 eV in a CO₂ molecule, but these modes are found to show quite different energy-dependence in the resonance peak. This feature arises from the different interaction scheme for excitation to each mode, *i.e.*, the weak polarization interaction for excitation to the symmetric stretching mode, weak dipole interaction for excitation to the bending mode, and strong dipole interaction for excitation to the asymmetric stretching mode. The asymmetric stretching shows sharp increase in differential cross sections (DCSs) toward small angle scattering due to the strong dipole interaction which washes out resonance features appeared at intermediate angles. DCSs for the symmetric and bending modes clearly show conspicuous isotropic features around 3.8 eV, thus emerging a sharp resonance.

I-M-2 Strong Suppression of Positronium Formation in Fluorinated Hydrocarbons in Positron Scattering: A Possibility of Bound States

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Strong suppression in positronium (Ps) formation is observed, for the first time, in fluorinated hydrocarbons. The reduction in Ps-formation cross sections is significantly pronounced, and the Ps-formation cross sections for fluorinated hydrocarbons (CF₄, C₂F₆, C₃F₈) are smaller by a factor of four-to-five than those for hydrocarbon counterparts (CH₄, C₂H₆, C₃H₈). This finding is a strong indication for the existence of bound states in fluorinated hydrocarbons because the high electronegativity of F atoms form F⁻ ions, and this in turn attracts positrons and forms a bound state near the edge of the charge distribution, thus reducing Ps formation.

I-M-3 Electron Capture in Collisions of Protons with CO Molecules in the keV Region: The Steric Effect

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Electron capture resulting from collisions of H⁺ ions with CO molecules has been investigated based on the molecular representation within the fully quantum mechanical formalism below 10 keV/u. Three different molecular configurations have been considered for collision dynamics, *i.e.*, (i) the proton approaches the center of mass of the CO molecule in the perpendicular configuration, (ii) the proton approaches the C atom in the collinear configuration, and (iii) the proton approaches the O atom in the collinear configuration. Electron capture dynamics and corresponding capture cross sections depend very sensitively on the molecular configuration, thus revealing a strong steric effect. The capture cross section from the CO electronic ground state is about 1.3×10^{-15} cm² at 10 keV/u, which is in good agreement with experimental findings. Differential cross sections (DCS's) for three molecular orientations have been examined both for elastic and electron capture processes, and the DCS averaged over all the configurations was found to agree well with a measurement from 0.02° to 1° at 1.5 keV/u.

I-M-4 The Isomer Effect on Charge Transfer: Collisions of Ground State C⁺ Ions with Allene and Propyne (C₃H₄)

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The isomer effect on charge transfer in collisions of C⁺ ions with allene and propyne (C₃H₄) molecules has been observed for the first time experimentally in the collision energy from 0.15 keV to 4.5 keV. In the present experiment, the ground state C⁺ (²P) ion projectiles have been produced by carefully energy-controlled electron impact to minimize the influence of the metastable-state ions. The observed cross sections are found that charge transfer cross sections for allene are slightly larger than those of propyne below 1 keV, although the difference becomes smaller as the collision energy increases. Both cross sections gradually decrease from around 1×10^{-14} cm² to 3×10^{-15} cm² as the collision energy increases from 0.2 keV to 4 keV. Since the molecular size of both molecules is similar, the size effect does not influence strongly on the cross section, but electronic structure is expected to be responsible to this difference. The dipole moment of propyne is larger

by a factor of four than that of allene, which should cause the more pronounced effect on the dynamics at much lower collision energies.

I-M-5 Electron Capture and Excitation in Collisions of Si^{2+} Ions with He Atoms at Intermediate Energies

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We have investigated electron capture and excitation in collisions of Si^{2+} ions with He atoms in the collision energy range from 0.02 keV/u to 6 keV/u based on a molecular representation. Molecular states are determined by using the multireference single- and double excitation configuration interaction method. We have considered electron capture and excitation both by the ground singlet and metastable triplet Si^{2+} ions. The capture cross section by the ground singlet Si^{2+} ion increases with increasing collision energy, and reaches a value of $\sim 1.3 \times 10^{-16} \text{ cm}^2$, while that by the metastable triplet ion is found to be large with a magnitude of $4 \times 10^{-16} \text{ cm}^2$ at the highest energy studied. Weak, but conspicuous, oscillatory structures are found for both cases, which are due to multichannel interference. The present rate coefficient for the ground singlet Si^{2+} ion impact is found to be much smaller than those of the $[\text{Si}^{4+} + \text{He}]$ system earlier studied