Elastic scattering of positrons from Ne, Ar, CH_4, and SiH_4

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Theoretical cross sections for elastic scattering of positrons (e^+) from Ne, Ar, CH_4, and SiH_4 targets have been reported. The latter two molecules belong to the Td point group, and effects of molecular anisotropy in these collision systems are rather small. The present theory is an extension of the previous work on electron-molecule collisions.[1] It is interesting to understand theoretically how the cross section for each target depends on the target property. Furthermore, the present work has also been stimulated by the experimental elastic differential cross sections (DCSs) which have been recently reported for CH_4[2] and Ar[3] over a large range of scattering angles of 30°–135°.

The present work is based on the fixed-nuclei approximation.[1] The interaction potential between a positron and a target is represented in the form of a local potential which consists of the electrostatic and the polarization potentials. As for the latter potential, a parameter-free model potential which is based on an electron-positron correlation energy in a homogeneous electron gas[4] is adopted for the smaller values of the positron-target distance, $\mathbf{r}$. This potential is connected with the long-range asymptotic form of the dipole polarization potential $-\alpha/2r^4$, where α denotes the dipole polarizability of target. The wavefunction of the scattered positron satisfies a set of coupled differential equations derived from the Schrödinger equation for the total collision system. By solving these equations, the scattering matrix is obtained from the asymptotic form of the wavefunction, and is transformed into the cross sections. Throughout the present calculation, no positronium (Ps) formation channel is taken into account.

The present calculations are carried out below the Ps formation threshold energy (E_{Ps}). E_{Ps} is given by $I - 6.8$ eV with I the first ionization potential, and is therefore obtained to be 14.76, 8.96, 5.8 and 4.8 eV for Ne, Ar, CH_4 and SiH_4, respectively. Figure 1 shows integral cross sections (ICSs) of the four collision systems as functions of collision energy. The present ICS for Ne is very good agreement with the measured total cross section (TCS).[5] As E_{Ps} becomes smaller however, a disagreement between the present elastic ICS and the experimental TCS[5] grows larger. The result suggests that an effect of Ps formation channel should play an important role in cross sections, particularly when E_{Ps} is small. As for Ne, a minimum is seen at around 0.8 eV. This mimimum is called the Ramsauer-Townsend one and is caused by a phase shift being very small from a dominant partial wave component. The minimum gradually disappears as target moves on from Ne to SiH_4 both experimentally and theoretically. This result is easily explained as follows. The interaction potential is, in the asymptotic region of $\mathbf{r}$, described by an attractive polarization potential which is proportional to the value of α, that is, 2.66, 11.10, 17.97, and 30.40 au for Ne, Ar, CH_4, and SiH_4, respectively. That is why, as magnitude of α is larger, superposition of higher partial wave components is more complicated and the minimum becomes more ambiguous.

The elastic DCSs for Ne, Ar, CH_4 and SiH_4 are shown in Fig. 2. Since the measured DCSs for Ar and CH_4 are in a relative scale, they are normalized at a scattering angle of 90° to the values of the respective present DCSs. The present DCS for each target has a notable minimum at around 40–50°, and its position moves to be at smaller angle as the energy

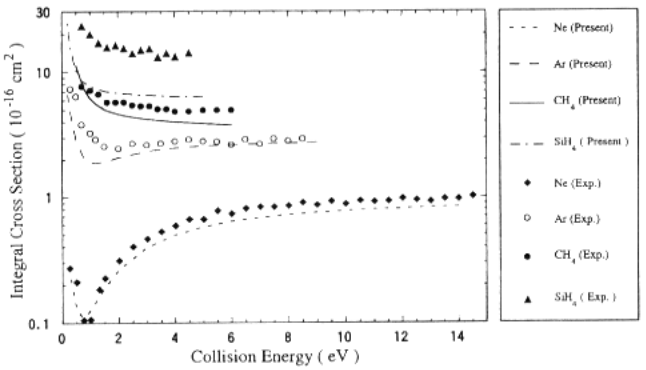

Fig. 1. Integral cross sections for positrons scattered from Ne, Ar, CH_4, and SiH_4. Comparisons are made with the experimental total cross sections.[5]

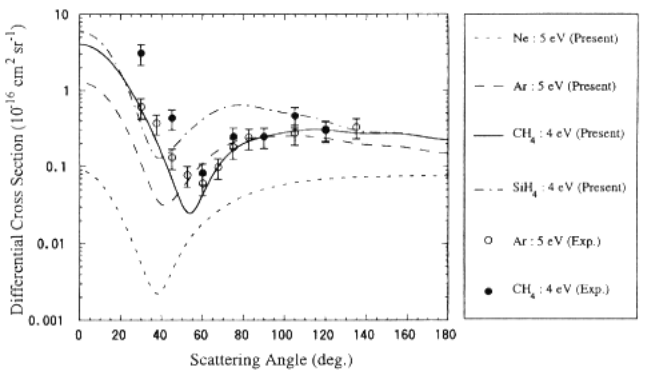

Fig. 2. Differential cross sections for positrons scattered from Ne, Ar, CH_4, and SiH_4. Comparisons are made with the experimental differential cross sections for Ar[3] and CH_4.[2]

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increases, which is probably due to the rainbow scattering caused by the repulsive electrostatic and the attractive polarization interaction potential terms. In the case of Ar and CH_4, the shapes of the present DCSs are generally in good agreement with the measured ones.[2,3] We have also found similarity between the present DCSs for CH_4 and Ar not only in shape but also in magnitude. This may be attributed to a quantitative similarity between the interaction potentials for the two collision systems at asymptotic values of **r**.

References

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