A THEORETICAL STUDY ON ON e^-–CH_3 COLLISIONS IN THE LOW ENERGY RANGE

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The interest on electron collisions with highly reactive radicals such as CH_x, CF_x, (x= 1,2,3), etc, has grown recently, in view of their importance in the development of plasma devices. In particular, various cross sections of e^-–CH_3 collisions are expected to be important for the understanding and modelling of the chemistry in both planetary atmospheres and discharge plasmas.

Unfortunately, experimental determination of such cross sections for e^--radical collisions are difficult. Only very recently, limited electron-impact ionisation cross sections of a few molecular radicals were reported in the literature. For e^--CH_3 collisions, just two theoretical investigations were reported [1, 2]. In those works, total (TCS) and total absorption (TACS) cross sections in the (20-3000)-eV range were calculated.

In this work we present a theoretical study on elastic electron scattering by CH_3. Calculated cross sections for electron impact energies ranging from 0.1 to 30 eV are presented. In our calculation, the electron-molecule scattering dynamics is represented by an interaction potential (V^{SEP}) formed by the static, the exchange and the correlation-polarization contributions:

$$V^{SEP}(\vec{r}) = V_{st}(\vec{r}) + V_{ex}(\vec{r}) + V_{cp}(\vec{r}). \quad (1)$$

The iterative Schwinger variational method [3] is used to solve the scattering equations.

Fig. 1 shows our calculated integral cross sections (ICS's) for elastic e^-–CH_3 collision, in the (0.1–30)-eV range. The calculated ICS's for e^-–CH elastic scattering [4] as well as calculated [5] and experimental ICS's [6–8] for e^-–CH_4 are also shown for comparison. The minimum seen at around 0.3 eV in our data was identified as a Ramsauer-Townsend minimum. Additional results and discussion will be presented at the Symposium.

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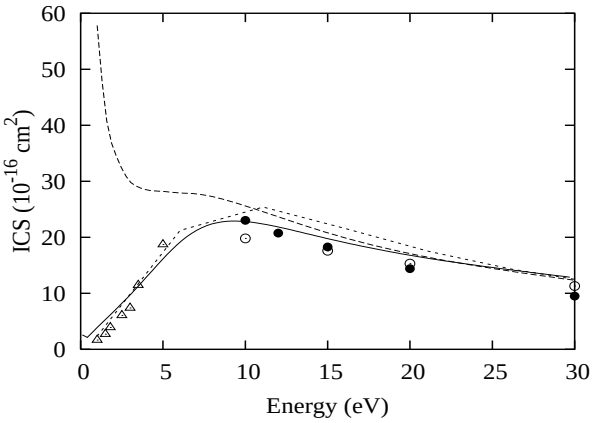

Fig. 1. ICS's for elastic e^-–CH_3 scattering in the (0.1-30)-eV energy range. Full curve, present calculated data; dashed line, calculated data for e^-–CH collisions [4]; short-dashed line, calculated ICS's for e^-–CH_4 [5]. Experimental results for e^-–CH_4 are: full circles, Boesten and Tanaka [6]; open circles, Shyn and Cravens [7]; open triangles, Sohn *et al* [8].

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