§4. Cross Section Database for Proton Charge Transfer Reactions with Hydrocarbon Molecules

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In most presently operating medium- and large-size fusion devices the plasma facing components in the divertor (divertor plates and side walls) contain carbon-based materials (graphite, carbon-carbon composites, etc.). The interaction of divertor hydrogenic plasma with these materials generates significant amounts of hydrocarbon molecules (mainly by chemical erosion) that enter the plasma. The composition of these fluxes depends on the energy of hydrogenic particles bombarding the carbon surfaces and on the surface temperature [1]. At bombarding energies in the range 30 - 500 eV, the lighter hydrocarbons, such as CH_3, CH_4 and C_2H_2, are preferentially formed, while with decreasing the impact energy towards 1 – 10 eV, heavier hydrocarbon molecules, such as C_2H_4, C_2H_6, C_3H_4, C_3H_6 and C_3H_8, become Increasingly dominant in the hydrocarbon fluxes from the walls. Once in the plasma, these molecules are subjected to various collision processes with plasma electrons and protons. Most of these processes lead to dissociation of reacting molecule and result in generation of all types of hydrocarbon molecules C_xH_y, independent of the composition of original erosion influxes. (Obviously, x and y should be smaller than x_{max} and y_{max} of the most complex CxHy molecule coming from the walls.)

The proton impact charge transfer reactions with hydrocarbon molecules

$$H^+ + C_xH_y \rightarrow H + C_xH_y^+ \qquad (1)$$

At the collision energies pertinent to divertor plasma temperatures (0.5 – 20 eV), the charge transfer reactions have significant cross sections, particularly when the number of hydrogen atoms in the molecule is large. This is mainly due to the large values of polarizabilities of hydrocarbon molecules, the exothermic character of reaction (1) for all CxHy molecules and the existence of internal degrees of freedom (vibrational and rotational) of $C_xH_y^+$ product ions, which can absorb the reaction exothermicity. This last circumstance facilitates the fulfillment of energy resonance condition for the reaction, resulting in a large value of its cross section.

In an effort to establish a complete database for the cross sections of reactions (1) with x = 1 – 3 and $y \leq 2x + 2$, we have compiled and critically assessed the sparse experimental and theoretical cross section data from the literature, and on their basis derived semi-empirical cross section scaling laws to generate the unavailable cross sections for most of the reactions of type (1). For the molecules C_xH_y with $y \geq 2x-2$, it was found that reaction (1) in the energy region below ~ 20 keV has a resonant character, with cross section of the order of magnitude 10^{-15} cm^2 (and larger in the eV region). For $y < 2x-2$, the resonant condition for the reaction (1) is not fulfilled and the corresponding cross sections are relatively small. However, the large polarizabilities of C_xH_y molecules nevertheless ensure large cross sections ($\geq 10^{-16}$ cm^2) in the sub-eV energy region even for this case.

The generated proton charge transfer cross section database for all C_xH_y ($x = 1$-3, $1 \leq y \leq 2x+2$) has been published in Ref.2.

References

1) Haasz, A.A. et al., Atom. Plasma-Mater. Int. Data Fusion, 7, (Part A) 5 (1998).
2) Janev, R.K. Kato, T., Wang, J.G., NIFS – DATA, **64** (2001).