

# 1 Addition 4: Adding I-DI cross sections for $C$ , $C_2$ , $C_3$

June 2006

Fits for the cross sections  $\sigma(E)$  for the ionization and dissociative ionization (I-DI) processes in the database [1, 2] have been given for  $C_xH_y$ ,  $x = 1, 2, 3$ ,  $y = 1, \dots, 2x + 2$ . In this present addition no. 4 we add the cross section data for  $C$ ,  $C_2$ ,  $C_3$  pure carbon atom and molecules, respectively. In particular the  $C_2$  density resulting from the breakup-chain from ethane or propane has been overestimated in previous applications of the HYDKIN online analysis tool, because the lifetime of  $C_2$  was overestimated due to lack of data for  $C_2$  destruction by dissociative ionization in the database [2].

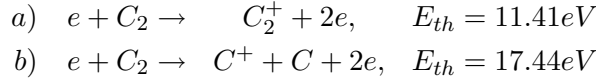
## 1.1 C

## 1.2 $C_2$

The fitting coefficients for Eq. (47)

$$\sigma_{ion} = \frac{10^{-13}}{E \cdot I_c} \left[ A_1 \ln \left( \frac{E}{I_c} \right) + \sum_{j=2}^N A_j \left( 1 - \frac{I_c}{E} \right)^{j-1} \right] \quad (cm^2) \quad (1)$$

for cross sections for the two channels



mentioned in [2] were not given there in Appendix A1. Also they could not be constructed from the information given in that report: Although the ‘‘universal I-DI formula’’ Eqs. (48, 49, 50) for the total cross section

$$\sigma_{ion}^{tot}(C_2H_y) = A_0 F_2^{ion}(y) \left( 1 - \frac{E_{th}}{E} \right)^\alpha \frac{1}{E} \ln(e + cE) \quad (\times 10^{-16} cm^2) \quad (2)$$

with

$$A_0 = 84.0, \quad \alpha = 3.0, \quad c = 0.09, \quad F_2^{ion}(y) = 2.97 + 0.073y$$

could, in principle, be employed (here with  $y = 0$ ), the branching ratios  $R_{I,DI}$  to obtain the partial cross sections have not been given in Table 4 of [2] (whereas those for the  $C_3$  DI processes have been given).

Employing this ‘‘universal’’ formula for the total cross section with  $y = 0$ , and using the estimate (see Eq. (36), with  $\alpha = 2$ , which is more appropriate in the 80 eV region than the  $\alpha = 3$  value mentioned above for the near threshold region):

$$\frac{\sigma_a(80eV)}{\sigma_b(80eV)} \simeq \left( \frac{E_{th}^{(b)}}{E_{th}^{(a)}} \right)^2 \quad (3)$$

we find  $R_I^a = 0.7003$  and  $R_{DI}^b = 0.2997$ .

Hence we can estimate the partial cross sections as (E in eV):

$$\begin{aligned}\sigma^a(E) &= 174.71 \left(1 - \frac{11.41}{E}\right)^3 \frac{1}{E} \ln(e + 0.009E) \quad (\times 10^{-16} \text{ cm}^2) \\ \sigma^b(E) &= 74.77 \left(1 - \frac{17.44}{E}\right)^3 \frac{1}{E} \ln(e + 0.009E) \quad (\times 10^{-16} \text{ cm}^2)\end{aligned}$$

These two cross sections have also been fitted into the format of Eq. (1) and the fitting coefficients are given in table ?? of addition no. 3 (which is the revision of table A1 in the Appendix of [2]). After this the total cross section  $\sigma(C_2) = \sigma^a(C_2) + \sigma^b(C_2)$  has been also been fitted with expression (1), and again these fitting coefficients are given in the revised version of table A1 in addition no. 3.

### 1.3 C<sub>3</sub>

## References

- [1] R. K. Janev and D. Reiter, *Phys. Plasmas* *9*, 4071(2002); see also: R. K. Janev and D. Reiter: "Collision processes of hydrocarbon species in hydrogen plasmas: I. The methane family", Report FZ-Jülich Jül-3966, Forschungszentrum Jülich, Jülich Germany (Feb. 2002).
- [2] R. K. Janev and D. Reiter, *Phys. Plasmas* *11*, 780 (2004); see also: R. K. Janev and D. Reiter, "Collision processes of hydrocarbon species in hydrogen plasmas: II. The ethane and propane families", Report FZ-Jülich Jül-4005, Forschungszentrum Jülich, Jülich Germany (Oct. 2002).