– Supplementary material –

Production of neutral species in Titan's ionosphere through dissociative recombination of ions

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1 The Database

Models of ion-neutral chemistry generally include DR processes through the reaction rate constant

$$\alpha(T_e) = \alpha_0 \times (T_e/T_0)^{-\beta} \tag{1}$$

where α_0 is the rate constant at a reference electron temperature T_0 (typically 300 K), and T_e is the electron temperature of interest. When more than one product channel is accessible, the partial rate for channel i is $\alpha_i(T_e) = b_i \times \alpha(T_e)$, where $\{b_i, i = 1, N\}$ are the *branching ratios* of the reaction. As the global DR rate $\alpha(T_e)$ and the branching ratios $\{b_i\}$ are typically derived from different experiments, they are treated separately.

The following tables report data for ions identified in Titan's ionosphere. **At the present stage, this is a demonstration database for the use of Nested Dirichlet representations of uncertain branching ratios, and it should not be considered or used as a reference database without caution**.

1.1 Rate constant parameters

The procedure for data representation as probability density functions is explained in the main paper.

1.2 Branching ratios

Information on branching ratios is typically sparser than for reaction rates, and it is exceptional to have to consider conflicting data. The following set of considerations is used in order to define the structures of the (Nested) Dirichlet distributions.

Maximum number of fragments. In absence of experimentally characterized products, one should consider all the exoergic channels and state a total lack of knowledge on the corresponding branching ratios (Diun distribution). It is not possible to make further hypotheses wrt. the relative stability of the products. From Ref. [1], we know for instance that the measured branching ratios have no definite correlation with the exoergicity of the pathways. An issue in building a list of exoergic pathways is the number of fragments that can be accepted in each pathway. For instance, on the basis of their previous results, for $C_3H_7^+$ Ehlerding *et al.*[2] stop at a three body breakup pattern, even though some four body channels are opened (C_3H_3 + H_2 + 2 H, C_2H_2 + CH_3 + 2 H). Other authors consider also four body breakup patterns in their analysis: CD_3CDO^+,[3] CD_3CND^+,[4] and CH_2CHCNH^+.[5] In the present treatment, we favored an exhaustive treatment and we enabled four body breakups when possible.

H_2 *vs.* 2H. An empirical rule appears throughout the database of branching ratios: the loss of 2 H atoms is more – often much more – probable than the loss of an H_2 molecule. The only measured exception is NH_4^+. This rule is used to reduce uncertainty by nesting both pathways using a Dior distribution.

Heavy fragments as a basis for nesting. A corrolary of the previous rule is that we are often induced to nest together pathways involving the same heavy fragment (e.g. X + 2H and X + H_2). For hydrocarbons, and in absence of experimental values, we adopted this as a general guideline to ensure a balanced treatment amongst those heavy fragments. This rule becomes ambiguous for N-bearing molecules and was restricted to hydrocarbon ions.

Spin states. Some species in the photochemical model have specified spin states. This is mostly the case for CH_2 and N. When the spin states of DR products have not been measured, we nest them inside a uniform Dirichlet subtree.

An overall view of the database content is provided in Fig. 1

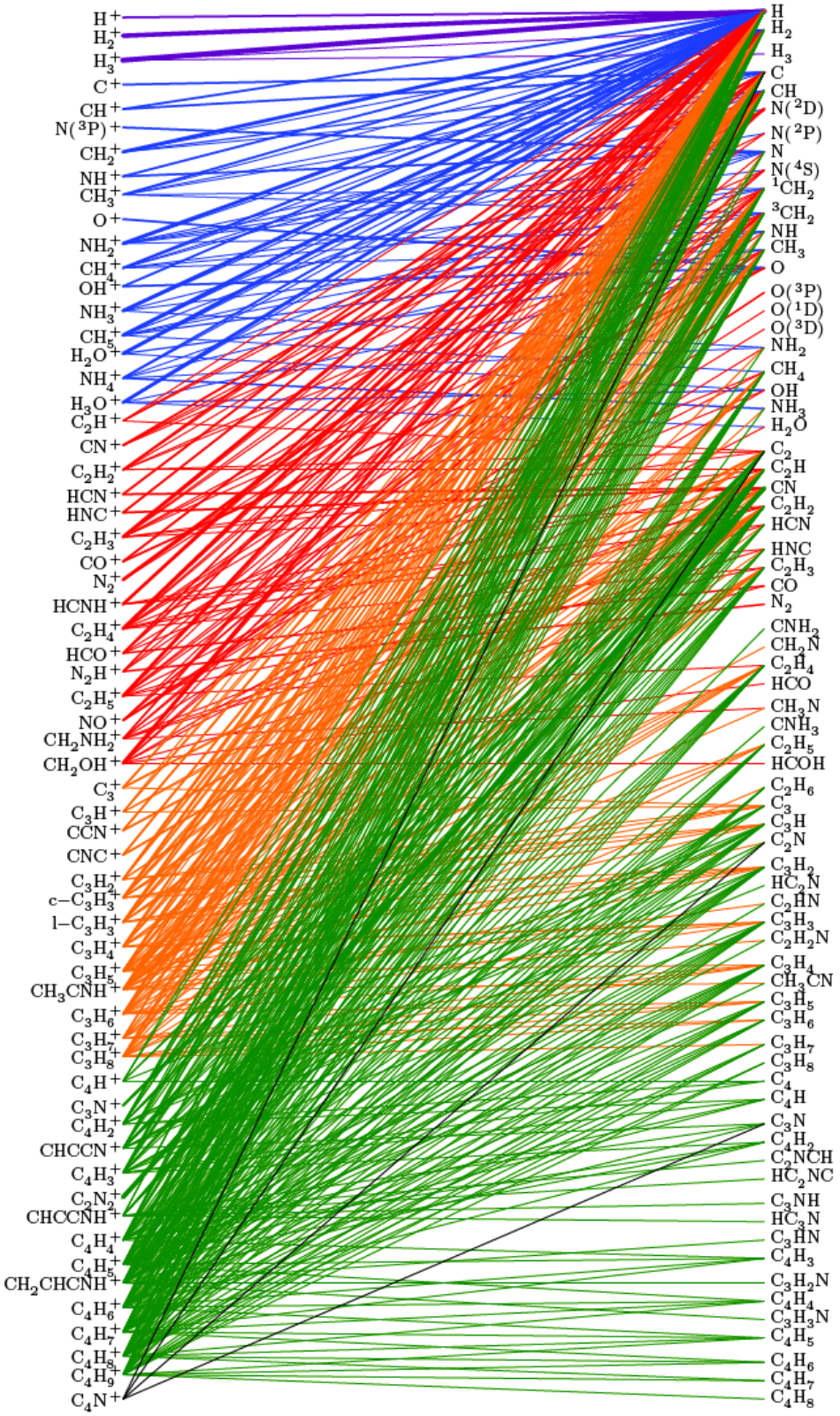

Figure 1: Representation of the fragmentation patterns for all ions treated in the present dataset. The line width is proportional to the production rate of the corresponding neutral, normalized to the rate constant. The colors depict the number of heavy atoms in the original ion.

Table 1: DR database

reaction		$\alpha_0(cm^3.s^{-1})$	$F_{\alpha_0} = 1 + \frac{u(\alpha_0)}{\alpha_0}$	β	$\frac{u(\beta)}{\beta}$	b
$H^+ + e^-$	$\rightarrow H$	1.6×10^{-6} [this work]	2 [this work]	0.5 – 1.5 [this work]	-	-
$H_2^+ + e^-$	$\rightarrow 2\,H$	1.6×10^{-6} [1]	2 [this work]	0.43 [1]	1 [this work]	-
$H_3^+ + e^-$	$\rightarrow H_3$	7.2×10^{-8} [6–8]	1.15 [6–8]	$0.48 - 1.0$ [1, 9–11]	-	$0.00 - 0.09$ [1]
	$\rightarrow H_2 + H$					$0.25 - 0.40$ [1, 10]
	$\rightarrow 3\,H$					$0.51 - 0.75$ [1, 10]
$C^+ + e^-$	$\rightarrow C + h\nu$	4.67×10^{-12} [12, 13]	1.5 [13]	0.6 [13]	0.5 [Woodall et al. [13]]	-
$CH^+ + e^-$	$\rightarrow C + H$	$0.97 - 3.1 \times 10^{-7}$ [1, 13–15]		0.37 – 0.89 [1, 13–15]	-	-
$CH_2^+ + e^-$	$\rightarrow CH + H$	$2.5 - 8.7 \times 10^{-7}$ [14, 16]	-	0.50 – 0.60 [14, 16]	-	0.25 ± 0.04 [16]
	$\rightarrow C + H_2$					0.12 ± 0.02 [16]
	$\rightarrow C + 2\,H$					0.63 ± 0.06 [16]
$CH_3^+ + e^-$	$\rightarrow \begin{cases} {}^1CH_2 + H \\ {}^3CH_2 + H \end{cases}$	$3.56 - 12.0 \times 10^{-7}$ [1, 14, 15]	-	0.51 [1, 14, 15]	0.04 [1, 14, 15]	0.40 ± 0.1 [17]
	$\rightarrow CH + H_2$					0.14 ± 0.1 [17]
	$\rightarrow CH + 2\,H$					0.16 ± 0.15 [17]
	$\rightarrow C + H_2 + H$					0.30 ± 0.08 [17]
$CH_4^+ + e^-$	$\rightarrow \begin{cases} CH_3 + H \\ \begin{cases} \begin{cases} {}^1CH_2 + H_2 \\ {}^3CH_2 + H_2 \end{cases} \\ \begin{cases} {}^1CH_2 + 2\,H \\ {}^3CH_2 + 2\,H \end{cases} \end{cases} \\ \begin{cases} CH + H_2 + H \\ CH + 3\,H \end{cases} \\ C + 2\,H_2 \end{cases}$	$3.5 - 12.8 \times 10^{-7}$ [1, 14, 15]	-	0.51 [1, 14, 15]	0.04 [1, 14, 15]	$0 - 1$ [this work]

Table 1: DR database *cont'd*

reaction	$\alpha_0(cm^3.s^{-1})$	$F_{\alpha_0} = 1 + \frac{u(\alpha_0)}{\alpha_0}$	β	$\frac{u(\beta)}{\beta}$	b
$CH_5^+ + e^-$					
$\rightarrow CH_4 + H$	$2.8 - 14 \times 10^{-7}$ [1, 14, 15, 18–22]	-	0.3−1 ($T_e \leq 300$ K); 1.5 ($T_e \geq 300$ K) [1, 14, 15, 18, 21, 22]	1 ($T_e \geq 300$ K) [this work]	0.049 ± 0.013 [21]; 0.95 ± 0.05 [23]
$\rightarrow CH_3 + H_2$ (a)					0.048 ± 0.002 [21]; (a) + (b) ≤ 0.08 [23]
$\rightarrow CH_3 + 2\,H$ (b)					0.698 ± 0.008 [21]; (a) + (b) ≤ 0.08 [23]
$\rightarrow \begin{cases} {}^1CH_2 + H_2 + H \\ {}^3CH_2 + H_2 + H \end{cases}$					0.172 ± 0.016 [21]; ≤ 0.01 [23]
$\rightarrow CH + 2\,H_2$					0.033 ± 0.011 [21]; ≤ 0.01 [23]
$C_2H^+ + e^-$					
$\rightarrow C_2 + H$	2.7×10^{-7} [1, 24]	1.26 [24]	0.76 [1, 15, 24]	0.33 [1, 15, 24]	0.43 ± 0.03 [24]
$\rightarrow CH + C$					0.39 ± 0.04 [24]
$\rightarrow 2\,C + H$					0.18 ± 0.04 [24]
$C_2H_2^+ + e^-$					
$\rightarrow C_2H + H$	$2.7 - 10 \times 10^{-7}$ [1, 15]	-	$0.5 - 1$ [1, 15]	-	0.50 ± 0.06 [25]
$\rightarrow C_2 + 2\,H$					0.30 ± 0.05 [25]
$\rightarrow C_2 + H_2$					0.02 ± 0.03 [25]
$\rightarrow \begin{cases} {}^1CH_2 + C \\ {}^3CH_2 + C \end{cases}$					0.05 ± 0.01 [25]
$\rightarrow 2\,CH$					0.13 ± 0.01 [25]
$C_2H_3^+ + e^-$					
$\rightarrow C_2H_2 + H$	$4.5 - 16 \times 10^{-7}$ [1, 15, 26, 27]	-	0.84 ($T_e \leq 800$ K) [1, 15, 26, 27]; $1.38 - 1.5$ ($T_e \geq 800$ K) [26, 27]	0.3 (T<800 K) [1, 15, 26, 27]	0.29 ± 0.04 [26]
$\rightarrow C_2H + H_2$					0.06 ± 0.03 [26]
$\rightarrow C_2H + 2\,H$					0.584 ± 0.06 for $\sum = 1$ (0.59) [26]
$\rightarrow C_2 + H + H_2$					0.03 ± 0.01 [26]
$\rightarrow CH_3 + C$					0.006 ± 0.002 [26]
$\rightarrow \begin{cases} {}^1CH_2 + CH \\ {}^3CH_2 + CH \end{cases}$					0.03 ± 0.01 [26]

Table 1: DR database *cont'd*

reaction	$\alpha_0(cm^3.s^{-1})$	$F_{\alpha_0} = 1 + \frac{u(\alpha_0)}{\alpha_0}$	β	$\frac{u(\beta)}{\beta}$	b
$C_2H_4^+ + e^-$					
$\rightarrow C_2H_3 + H$	5.6×10^{-7} [24]	1.11 [24]	0.76 [24, 27]	1 [this work]	0.11 ± 0.07 [24]
$\rightarrow C_2H_2 + H_2$					0.06 ± 0.03 [24]
$\rightarrow C_2H_2 + 2\,H$					0.66 ± 0.06 [24]
$\rightarrow C_2H + H_2 + H$					0.10 ± 0.04 [24]
$\rightarrow CH_4 + C$					0.01 ± 0.01 [24]
$\rightarrow CH_3 + CH$					0.02 ± 0.02 [24]
$\rightarrow \begin{cases} {}^1CH_2 + {}^1CH_2 \\ {}^1CH_2 + {}^3CH_2 \\ {}^3CH_2 + {}^3CH_2 \end{cases}$					0.04 ± 0.02 [24]
$C_2H_5^+ + e^-$					
$\rightarrow C_2H_4 + H$	8.35×10^{-7} [1, 19, 20, 22]	1.30 [1, 19, 20, 22]	0.8 ($T_e \leq 300$ K) [22]; 1.2 ($T_e \geq 300$ K) [22]	1 [this work]	0.12 ± 0.03 [28]
$\rightarrow C_2H_3 + 2\,H$					0.27 ± 0.04 [28]
$\rightarrow C_2H_2 + 3\,H$					0.13 ± 0.03 [28]
$\rightarrow C_2H_2 + H_2 + H$					0.30 ± 0.03 for $\sum = 1$ (0.29) [28]
$\rightarrow \begin{cases} CH_3 + {}^1CH_2 \\ CH_3 + {}^3CH_2 \end{cases}$					0.17 ± 0.01 [28]
$\rightarrow CH_4 + CH$					0.01 ± 0.01 [28]
$C_3^+ + e^-$					
$\rightarrow C_3$	$0.5 - 3 \times 10^{-6}$ [this work]	-	0.5 – 1.5 [this work]	-	0.000 ± 0.001 [27, 29]
$\rightarrow C_2 + C$					1.000 ± 0.002 [27, 29]
$\rightarrow 3\,C$					0.000 ± 0.001 [27, 29]
$C_3H^+ + e^-$					
$\rightarrow C_3 + H$	$0.5 - 3 \times 10^{-6}$ [this work]	-	0.5 – 1.5 [this work]	-	0.662 ± 0.015 [1, 15, 30, 31]
$\rightarrow C_2H + C$					0.338 ± 0.017 [1, 15, 30, 31]
$\rightarrow C_2 + CH$					0.00 ± 0.01 [1, 15, 30, 31]

Table 1: DR database *cont'd*

reaction	$\alpha_0(cm^3.s^{-1})$	$F_{\alpha_0} = 1 + \frac{u(\alpha_0)}{\alpha_0}$	β	$\frac{u(\beta)}{\beta}$	b
$C_3H_2^+ + e^-$					
$\rightarrow \begin{cases} \begin{cases} C_3 + H_2 \\ C_3 + 2\,H \end{cases} \\ C_3H + H \end{cases}$	$0.5 - 3 \times 10^{-6}$ [this work]	-	0.5 – 1.5 [this work]	-	0.875 ± 0.017 [1, 15, 30, 31]
$\rightarrow \begin{cases} C_2H + CH \\ C_2H + C + H \end{cases}$					0.125 ± 0.021 [1, 15, 30, 31]
$c - C_3H_3^+ + e^-$					
$\rightarrow \begin{cases} C_3H_2 + H \\ \begin{cases} C_3H + H_2 \\ C_3H + 2\,H \end{cases} \\ C_3 + H + H_2 \end{cases}$	8.00×10^{-7} [32]	1.0125 [32]	0.0 [1, 15, 27]	$\sigma_n = 0.7$ [1, 15, 27]	0.907 ± 0.011 [1, 15, 30, 31]
$\rightarrow \begin{cases} \begin{cases} C_2H_2 + CH \\ C_2H_2 + C + H \end{cases} \\ \begin{cases} C_2H + {}^1CH_2 \\ C_2H + {}^3CH_2 \end{cases} \\ C_2 + CH_3 \end{cases}$					0.093 ± 0.005 [1, 15, 30, 31]
$l - C_3H_3^+ + e^-$					
$\rightarrow \begin{cases} C_3H_2 + H \\ \begin{cases} C_3H + H_2 \\ C_3H + 2\,H \end{cases} \\ C_3 + H + H_2 \end{cases}$	1.15×10^{-7} [1, 15, 27, 32]	1.17 [32]	0.0 [1, 15, 27]	$\sigma_n = 0.2$ [1, 15, 27]	0.907 ± 0.011 [1, 15, 30, 31]
$\rightarrow \begin{cases} \begin{cases} C_2H_2 + CH \\ C_2H_2 + C + H \end{cases} \\ \begin{cases} C_2H + {}^1CH_2 \\ C_2H + {}^3CH_2 \end{cases} \\ C_2 + CH_3 \end{cases}$					0.093 ± 0.005 [1, 15, 30, 31]
$C_3H_4^+ + e^-$					
$\rightarrow C_3H_3 + H$	2.95×10^{-6} [33]	1.034 [33]	0.67 [33]	0.03 [33]	0.87±0.04 [1, 15, 30, 31, 33]
$\rightarrow C_3H_2 + H_2$					≤0.02 [1, 15, 30, 31, 33]
$\rightarrow C_3H_2 + 2\,H$					≤0.05 [1, 15, 30, 31, 33]
$\rightarrow C_2H_3 + CH$					0.01 ±0.01 [1, 15, 30, 31, 33]

Table 1: DR database *cont'd*

reaction	$\alpha_0(cm^3.s^{-1})$	$F_{\alpha_0} = 1 + \frac{u(\alpha_0)}{\alpha_0}$	β	$\frac{u(\beta)}{\beta}$	b
$\rightarrow \begin{cases} C_2H_2 +^1 CH_2 \\ C_2H_2 +^3 CH_2 \end{cases}$					0.06 ± 0.02 [1, 15, 30, 31, 33]
$\rightarrow C_2H + CH_3$					0.01 ± 0.01 [1, 15, 30, 31, 33]
$C_3H_5^+ + e^-$ $\rightarrow \begin{cases} C_3H_4 + H \\ \begin{cases} C_3H_3 + H_2 \\ C_3H_3 + 2\,H \end{cases} \\ C_3H_2 + H_2 + H \\ C_3H + 2\,H_2 \end{cases}$	$0.5 - 3 \times 10^{-6}$ [this work]	-	0.5 – 1.5 [this work]	-	0.867 ± 0.004 [1, 15, 30, 31]
$\rightarrow \begin{cases} C_2H_5 + C \\ C_2H_4 + CH \\ \begin{cases} C_2H_3 +^1 CH_2 \\ C_2H_3 +^3 CH_2 \end{cases} \\ \begin{cases} \begin{cases} C_2H_2 +^1 CH_2 + H \\ C_2H_2 +^3 CH_2 + H \end{cases} \\ C_2H_2 + CH + H_2 \\ C_2H_2 + CH_3 \end{cases} \\ \begin{cases} C_2H + CH_3 + H \\ C_2H + CH_4 \end{cases} \end{cases}$					0.133 ± 0.026 [1, 15, 30, 31]
$C_3H_6^+ + e^-$ $\rightarrow \begin{cases} C_3H_5 + H \\ C_3H_4 + 2\,H \\ C_3H_3 + H_2 + H \\ \begin{cases} C_3H_2 + 2\,H_2 \\ C_3H_2 + H_2 + 2\,H \end{cases} \end{cases}$	$0.5 - 3 \times 10^{-6}$ [this work]	-	0.5 – 1.5 [this work]	-	0.693 ± 0.016 [1, 15, 30, 31]

Table 1: DR database *cont'd*

reaction	$\alpha_0(cm^3.s^{-1})$	$F_{\alpha_0} = 1 + \frac{u(\alpha_0)}{\alpha_0}$	β	$\frac{u(\beta)}{\beta}$	b
$\rightarrow$ $C_2H_5 + CH$					
$\rightarrow$ $C_2H_4 +^1 CH_2$					
$\rightarrow$ $C_2H_4 +^3 CH_2$					
$\rightarrow$ $C_2H_4 + CH + H$					
$\rightarrow$ $C_2H_4 + C + H_2$					
$\rightarrow$ $C_2H_3 + CH + H_2$					
$\rightarrow$ $C_2H_3 + CH_3$					0.307 ± 0.013 [1, 15, 30, 31]
$\rightarrow$ $C_2H_2 + CH_4$					
$\rightarrow$ $C_2H_2 +^1 CH_2 + H_2$					
$\rightarrow$ $C_2H_2 +^3 CH_2 + H_2$					
$\rightarrow$ $C_2H_2 + CH_3 + H$					
$\rightarrow$ $C_2H + CH_4 + H$					
$\rightarrow$ $C_2H + CH_3 + H_2$					
$C_3H_7^+ + e^-$ $\rightarrow$ $C + CH_2 + CH_4$					0.00 ± 0.01 [1, 15, 30, 31]
$C_3H_7^+ + e^-$ $\rightarrow$ $C_3H_6 + H$	$0.5-3\times10^{-6}$ [2, 19, 34]	-	0.68 [2]	0.015 [2]	0.13 ± 0.05 [34]
$\rightarrow$ $C_3H_5 + H_2$					0.12 ± 0.05 [34]
$\rightarrow$ $C_3H_5 + 2\,H$					0.22 ± 0.08 [34]
$\rightarrow$ $C_3H_4 + H_2 + H$					0.09 ± 0.02 [34]
$\rightarrow$ $C_2H_4 + CH_3$					0.03 ± 0.02 [34]
$\rightarrow$ $C_2H_3 + CH_4$					0.02 ± 0.02 [34]
$\rightarrow$ $C_2H_3 + CH_3 + H$					0.15 ± 0.04 [34]
$\rightarrow$ $C_2H_2 + CH_4 + H$					0.03 ± 0.03 [34]
$\rightarrow$ $C_2H_2 + CH_3 + H_2$					0.21 ± 0.04 [34]
$C_3H_8^+ + e^-$ $\rightarrow$ $C_3H_7 + H$	$0.5 - 3 \times 10^{-6}$ [this work]	-	0.5 – 1.5 [this work]	-	0.679 ± 0.029 [1, 15, 30, 31]
$\rightarrow$ $C_3H_6 + H_2$					
$\rightarrow$ $C_3H_6 + 2\,H$					
$\rightarrow$ $C_3H_5 + H_2 + H$					
$\rightarrow$ $C_3H_4 + 2\,H_2$					
$\rightarrow$ $C_3H_4 + H_2 + 2\,H$					

Table 1: DR database *cont'd*

reaction	$\alpha_0(cm^3.s^{-1})$	$F_{\alpha_0} = 1 + \frac{u(\alpha_0)}{\alpha_0}$	β	$\frac{u(\beta)}{\beta}$	b
$\rightarrow$ { $C_2H_6 +^1 CH_2$; $C_2H_6 +^3 CH_2$; $C_2H_5 + CH_3$ { $C_2H_5 +^1 CH_2 + H$; $C_2H_5 +^3 CH_2 + H$; $C_2H_5 + CH + H_2$; $C_2H_5 + CH + 2H$ }; $C_2H_4 + CH_4$; $C_2H_4 + CH_3 + H$ { $C_2H_4 +^1 CH_2 + H_2$ { $C_2H_4 +^1 CH_2 + 2H$; $C_2H_4 +^3 CH_2 + H_2$ { $C_2H_4 +^3 CH_2 + 2H$; $C_2H_3 + CH_3 + H_2$ { $C_2H_3 + CH_3 + 2H$; $C_2H_3 + CH_4 + H$; $C_2H_2 + CH_4 + H_2$					0.321 ± 0.028 [1, 15, 30, 31]
$\rightarrow$ { $CH_4 + CH_3 + CH$; $CH_4 +^1 CH_2 +^1 CH_2$; $CH_4 +^1 CH_2 +^3 CH_2$; $CH_4 +^3 CH_2 +^3 CH_2$; $2CH_3 +^1 CH_2$; $2CH_3 +^3 CH_2$ }					0.00 ± 0.01 [1, 15, 30, 31]
$C_4H^+ + e^-$ $\rightarrow C_4 + H$	$0.5 - 3 \times 10^{-6}$ [this work]	-	0.5 – 1.5 [this work]	-	0.439 ± 0.012 for $\sum = 1$ (0.438) [1, 31, 35]
$\rightarrow C_3H + C$					0.282 ± 0.021 [1, 31, 35]
$\rightarrow C_2H + C_2$					0.279 ± 0.017 [1, 31, 35]
$C_4H_2^+ + e^-$ $\rightarrow$ { $C_4H + H$; $C_4 + H_2$ }	$0.5 - 3 \times 10^{-6}$ [this work]	-	0.5 – 1.5 [this work]	-	0.783 ± 0.013 for $\sum = 1$ (0.784) [1, 31, 35]

Table 1: DR database *cont'd*

reaction	$\alpha_0(cm^3.s^{-1})$	$F_{\alpha_0} = 1 + \frac{u(\alpha_0)}{\alpha_0}$	β	$\frac{u(\beta)}{\beta}$	b
$\rightarrow \begin{cases} C_3H_2 + C \\ C_3H + CH \\ \begin{cases} C_3 +^1 CH_2 \\ C_3 +^3 CH_2 \end{cases} \end{cases}$					0.040 ± 0.016 [1, 31, 35]
$\rightarrow \begin{cases} C_2H_2 + C_2 \\ 2\,C_2H \end{cases}$					0.177 ± 0.015 [1, 31, 35]
$C_4H_3^+ + e^-$ $\rightarrow \begin{cases} C_4H_2 + H \\ \begin{cases} C_4H + H_2 \\ C_4H + 2\,H \end{cases} \\ C_4 + H + H_2 \end{cases}$	6.2×10^{-7} [1, 15, 36]	2 [this work]	0.5 − 1.5 [this work]	-	0.759 ± 0.005 for $\sum = 1$ (0.760) [1, 31, 35]
$\rightarrow \begin{cases} C_3H_3 + C \\ C_3H_2 + CH \\ \begin{cases} C_3H +^1 CH_2 \\ C_3H +^3 CH_2 \end{cases} \\ C_3 + CH_3 \end{cases}$					0.063 ± 0.004 [1, 31, 35]
$\rightarrow \begin{cases} C_2H_3 + C_2 \\ C_2H_2 + C_2H \end{cases}$					0.178 ± 0.004 [1, 31, 35]
$C_4H_4^+ + e^-$ $\rightarrow \begin{cases} C_4H_3 + H \\ \begin{cases} C_4H_2 + H_2 \\ C_4H_2 + 2\,H \end{cases} \\ C_4H + H_2 + H \end{cases}$	$0.5 - 3 \times 10^{-6}$ [this work]	-	0.5 − 1.5 [this work]	-	0.766 ± 0.027 [1, 31, 35]
$\rightarrow \begin{cases} C_3H_4 + C \\ C_3H_3 + CH \\ \begin{cases} \begin{cases} C_3H_2 +^1 CH_2 \\ C_3H_2 +^3 CH_2 \end{cases} \\ C_3H_2 + C + H_2 \end{cases} \\ C_3H + CH_3 \\ \begin{cases} C_3 + CH_4 \\ C_3 + CH_3 + H \end{cases} \end{cases}$					0.063 ± 0.02 [1, 31, 35]

Table 1: DR database *cont'd*

reaction	$\alpha_0(cm^3.s^{-1})$	$F_{\alpha_0} = 1 + \frac{u(\alpha_0)}{\alpha_0}$	β	$\frac{u(\beta)}{\beta}$	b
$\rightarrow \begin{cases} C_2H_4 + C_2 \\ C_2H_3 + C_2H \\ \begin{cases} 2\,C_2H_2 \\ C_2H_2 + C_2H + H \\ C_2H_2 + C_2 + H_2 \end{cases} \\ 2\,C_2H + H_2 \end{cases}$					0.171 ± 0.021 [1, 31, 35]
$C_4H_5^+ + e^-$ $\rightarrow \begin{cases} C_4H_4 + H \\ \begin{cases} C_4H_3 + H_2 \\ C_4H_3 + 2\,H \end{cases} \\ C_4H_2 + H_2 + H \\ C_4H + 2\,H_2 \end{cases}$	8.2×10^{-7} [37]	1.30 [37]	0.5 − 1.5 [this work]	-	0.460 ± 0.054 [1, 31, 35]
$\rightarrow \begin{cases} C_3H_5 + C \\ C_3H_4 + CH \\ \begin{cases} C_3H_3 +^1 CH_2 \\ C_3H_3 +^3 CH_2 \end{cases} \\ C_3H_2 + CH_3 \\ C_3H + CH_4 \end{cases}$					0.093 ± 0.021 [1, 31, 35]
$\rightarrow \begin{cases} C_2H_5 + C_2 \\ C_2H_4 + C_2H \\ C_2H_3 + C_2H_2 \\ \begin{cases} 2\,C_2H_2 + H \\ C_2H_2 + C_2H + H_2 \end{cases} \end{cases}$					0.447 ± 0.053 [1, 31, 35]
$C_4H_6^+ + e^-$ $\rightarrow \begin{cases} C_4H_5 + H \\ \begin{cases} C_4H_4 + H_2 \\ C_4H_4 + 2\,H \end{cases} \\ C_4H_3 + H_2 + H \\ \begin{cases} C_4H_2 + 2\,H_2 \\ C_4H_2 + H_2 + 2\,H \end{cases} \end{cases}$	$0.5 - 3 \times 10^{-6}$ [this work]	-	0.5 − 1.5 [this work]	-	0.589 ± 0.035 [1, 31, 35]

Table 1: DR database *cont'd*

reaction	$\alpha_0(cm^3.s^{-1})$	$F_{\alpha_0} = 1 + \frac{u(\alpha_0)}{\alpha_0}$	β	$\frac{u(\beta)}{\beta}$	b
$\rightarrow$ $C_3H_6 + C$					
$\rightarrow$ $C_3H_5 + CH$					
$\rightarrow$ $C_3H_4 + {}^1CH_2$					
$\rightarrow$ $C_3H_4 + {}^3CH_2$					
$\rightarrow$ $C_3H_4 + C + H_2$					
$\rightarrow$ $C_3H_3 + CH_3$					
$\rightarrow$ $C_3H_3 + CH + H_2$					0.090 ± 0.015 [1, 31, 35]
$\rightarrow$ $C_3H_2 + CH_4$					
$\rightarrow$ $C_3H_2 + CH_3 + H$					
$\rightarrow$ $C_3H_2 + {}^1CH_2 + H_2$					
$\rightarrow$ $C_3H_2 + {}^3CH_2 + H_2$					
$\rightarrow$ $C_3H + CH_4 + H$					
$\rightarrow$ $C_3H + CH_3 + H_2$					
$\rightarrow$ $C_2H_6 + C_2$					
$\rightarrow$ $C_2H_5 + C_2H$					
$\rightarrow$ $C_2H_4 + C_2H + H$					
$\rightarrow$ $C_2H_4 + C_2H_2$					0.321 ± 0.034 [1, 31, 35]
$\rightarrow$ $C_2H_4 + C_2 + H_2$					
$\rightarrow$ $C_2H_3 + C_2H_2 + H$					
$\rightarrow$ $C_2H_3 + C_2H + H_2$					
$\rightarrow$ $C_2H_2 + CH + CH_3$					0.00 ± 0.01 [1, 31, 35]
$\rightarrow$ $C_2H_2 + C + CH_4$					
$C_4H_7^+ + e^-$ $\rightarrow$ $C_4H_6 + H$	$0.5 - 3 \times 10^{-6}$ [this work]	-	$0.5 - 1.5$ [this work]	-	0.198 ± 0.044 [1, 31, 35]
$\rightarrow$ $C_4H_5 + H_2$					
$\rightarrow$ $C_4H_5 + 2H$					
$\rightarrow$ $C_4H_4 + H_2 + H$					
$\rightarrow$ $C_4H_3 + 2H_2$					

Table 1: DR database *cont'd*

reaction	$\alpha_0(cm^3.s^{-1})$	$F_{\alpha_0} = 1 + \frac{u(\alpha_0)}{\alpha_0}$	β	$\frac{u(\beta)}{\beta}$	b
$\rightarrow$ $C_3H_7 + C$ $C_3H_6 + CH$ $C_3H_5 +^1 CH_2$ $C_3H_5 +^3 CH_2$ $C_3H_4 + CH_3$ $C_3H_4 +^1 CH_2 + H$ $C_3H_4 +^3 CH_2 + H$ $C_3H_4 + CH + H_2$ $C_3H_3 + CH_4$ $C_3H_3 + CH_3 + H$ $C_3H_3 +^1 CH_2 + H_2$ $C_3H_3 +^3 CH_2 + H_2$ $C_3H_2 + CH_4 + H$ $C_3H_2 + CH_3 + H_2$ $C_3H + CH_4 + H_2$					0.655 ± 0.059 [1, 31, 35]
$\rightarrow$ $C_2H_6 + C_2H$ $C_2H_5 + C_2H_2$ $C_2H_4 + C_2H_2 + H$ $C_2H_4 + C_2H + H_2$ $2\,C_2H_3 + H$ $C_2H_3 + C_2H_2 + H_2$					0.147 ± 0.034 [1, 31, 35]
$\rightarrow$ $C_2H_2 +^1 CH_2 + CH_3$ $C_2H_2 +^3 CH_2 + CH_3$					0.00 ± 0.01 [1, 31, 35]
$C_4H_8^+ + e^-$ $\rightarrow$ $C_4H_7 + H$ $C_4H_6 + H_2$ $C_4H_6 + 2\,H$ $C_4H_5 + H_2 + H$ $C_4H_5 + 3\,H$ $C_4H_4 + 2\,H_2$ $C_4H_4 + H_2 + 2\,H$	$0.5 - 3 \times 10^{-6}$ [this work]	-	0.5 – 1.5 [this work]	-	0.305 ± 0.031 [1, 31, 35]

Table 1: DR database *cont'd*

reaction	$\alpha_0(cm^3.s^{-1})$	$F_{\alpha_0} = 1 + \frac{u(\alpha_0)}{\alpha_0}$	β	$\frac{u(\beta)}{\beta}$	b
$\rightarrow \begin{cases} C_3H_8 + C \\ C_3H_7 + CH \\ \begin{cases} \begin{cases} C_3H_6 +^1 CH_2 \\ C_3H_6 +^3 CH_2 \end{cases} \\ C_3H_6 + CH + H \\ C_3H_6 + C + H_2 \end{cases} \\ \begin{cases} C_3H_5 + CH_3 \\ \begin{cases} C_3H_5 +^1 CH_2 + H \\ C_3H_5 +^3 CH_2 + H \end{cases} \\ C_3H_5 + CH + H_2 \end{cases} \\ \begin{cases} C_3H_4 + CH_4 \\ C_3H_4 + CH_3 + H \\ \begin{cases} C_3H_4 +^1 CH_2 + H_2 \\ C_3H_4 +^3 CH_2 + H_2 \end{cases} \end{cases} \\ \begin{cases} C_3H_3 + CH_4 + H \\ C_3H_3 + CH_3 + H_2 \end{cases} \\ \begin{cases} C_3H_2 + CH_4 + H_2 \\ C_3H_2 + CH_4 + 2H \end{cases} \end{cases}$					0.634 ± 0.032 for $\sum = 1$ (0.635) [1, 31, 35]
$\rightarrow \begin{cases} \begin{cases} C_2H_6 + C_2H_2 \\ C_2H_6 + C_2H + H \\ C_2H_6 + C_2 + H_2 \end{cases} \\ \begin{cases} C_2H_5 + C_2H_3 \\ C_2H_5 + C_2H_2 + H \\ C_2H_5 + C_2H + H_2 \end{cases} \\ \begin{cases} 2\,C_2H_4 \\ C_2H_4 + C_2H_3 + H \end{cases} \end{cases}$					0.061 ± 0.021 [1, 31, 35]

Table 1: DR database *cont'd*

reaction	$\alpha_0(cm^3.s^{-1})$	$F_{\alpha_0} = 1 + \frac{u(\alpha_0)}{\alpha_0}$	β	$\frac{u(\beta)}{\beta}$	b
$\rightarrow \begin{cases} \begin{cases} C_2H_4 + CH + CH_3 \\ C_2H_4 + C + CH_4 \end{cases} \\ C_2H_3 + CH + CH_4 \\ \begin{cases} C_2H_2 + 2\,CH_3 \\ \begin{cases} C_2H_2 +^1 CH_2 + CH_4 \\ C_2H_2 +^3 CH_2 + CH_4 \end{cases} \end{cases} \\ C_2H + CH_4 + CH_3 \\ C_2 + 2\,CH_4 \end{cases}$					0.000 ± 0.010 [1, 31, 35]
$C_4H_9^+ + e^-$ $\rightarrow \begin{cases} C_4H_8 + H \\ \begin{cases} C_4H_7 + H_2 \\ C_4H_7 + 2\,H \end{cases} \\ C_4H_6 + H_2 + H \\ \begin{cases} C_4H_5 + 2\,H_2 \\ C_4H_5 + H_2 + 2\,H \end{cases} \end{cases}$	8.3×10^{-7} [19]	1.30 [19]	0.5 – 1.5 [this work]	-	0.574 ± 0.041 for $\sum = 1$ (0.575) [1, 31, 35, 38]
$\rightarrow \begin{cases} C_3H_8 + CH \\ \begin{cases} C_3H_7 +^1 CH_2 \\ C_3H_7 +^3 CH_2 \end{cases} \\ \begin{cases} C_3H_6 + CH_3 \\ \begin{cases} C_3H_6 +^1 CH_2 + H \\ C_3H_6 +^3 CH_2 + H \end{cases} \\ C_3H_6 + CH + H_2 \end{cases} \\ \begin{cases} C_3H_5 + CH_4 \\ C_3H_5 + CH_3 + H \\ \begin{cases} C_3H_5 +^1 CH_2 + H_2 \\ C_3H_5 +^3 CH_2 + H_2 \end{cases} \end{cases} \\ \begin{cases} C_3H_4 + CH_4 + H \\ C_3H_4 + CH_3 + H_2 \end{cases} \\ C_3H_3 + CH_4 + H_2 \end{cases}$					0.411 ± 0.038 [1, 31, 35, 38]

Table 1: DR database *cont'd*

reaction	$\alpha_0(cm^3.s^{-1})$	$F_{\alpha_0} = 1 + \frac{u(\alpha_0)}{\alpha_0}$	β	$\frac{u(\beta)}{\beta}$	b
$\rightarrow$ { { $C_2H_6 + C_2H_3$; $C_2H_6 + C_2H_2 + H$; $C_2H_6 + C_2H + H_2$ }; { $C_2H_5 + C_2H_4$; $C_2H_5 + C_2H_3 + H$; $C_2H_5 + C_2H_2 + H_2$ }; $2\,C_2H_4 + H$					0.015 ± 0.026 [1, 31, 35, 38]
$\rightarrow$ { { $C_2H_4 + CH + CH_4$; { $C_2H_4 +^1 CH_2 + CH_3$; $C_2H_4 +^3 CH_2 + CH_3$ } }; { $C_2H_3 + 2\,CH_3$; { $C_2H_3 +^1 CH_2 + CH_4$; $C_2H_3 +^3 CH_2 + CH_4$ } }; $C_2H_2 + CH_3 + CH_4$					0.000 ± 0.010 [1, 31, 35, 38]
$C_5H_3^+ + e^-$ → unknown	9×10^{-7} [39]	1.30 [39]	0.5 – 1.5[this work]	-	-
$C_5H_9^+ + e^-$ → unknown	9.5×10^{-7} [37]	1.32 [37]	0.5 – 1.5[this work]	-	-
$C_6H_4^+ + e^-$ → unknown	1.10×10^{-6} [37]	1.30 [37]	0.5 – 1.5[this work]	-	-
$C_6H_5^+ + e^-$ → unknown	1.10×10^{-6} [37]	1.30 [37]	0.5 – 1.5[this work]	-	-
$C_6H_6^+ + e^-$ → unknown	1.0×10^{-6} [39]	1.33 [39]	0.5 – 1.5[this work]	-	-
$C_6H_7^+ + e^-$ → unknown	2.4×10^{-6} [22]	1.37 [22]	0.5 – 1.5 [this work] ($T \leq T_1$); 1.3 ($T \geq T_1$) [22]; $T_1 \leq 300$ K	1 [this work]	-
$C_7H_5^+ + e^-$ → unknown	7.0×10^{-7} [39]	1.29 [39]	0.5 – 1.5[this work]	-	-

Table 1: DR database *cont'd*

reaction		$\alpha_0(cm^3.s^{-1})$	$F_{\alpha_0} = 1 + \frac{u(\alpha_0)}{\alpha_0}$	β	$\frac{u(\beta)}{\beta}$	b
$N^+ + e^-$	$\rightarrow N + h\nu$	4.0×10^{-12} [12, 13]	1.50 [12, 13]	0.58 [12, 13]	0.5 [12, 13]	-
$NH^+ + e^-$	$\rightarrow N + H$	4.33×10^{-8} [1, 13, 15]	2 [this work]	0.5 – 1.5[this work]	-	-
$NH_2^+ + e^-$	$\rightarrow N + H_2$	$0.5 - 10 \times 10^{-7}$ [this work]	-	0.5 – 1.5[this work]	-	0.04 ± 0.03 [40, 41]
	$\rightarrow NH + H$					0.38 ± 0.06 [40, 41]
	$\rightarrow \begin{cases} (^4S)N + 2\,H \\ (^2D)N + 2\,H \\ (^2P)N + 2\,H \end{cases}$					0.58 ± 0.09 $\begin{cases} 0.53 \pm 0.04 \\ 0.45 \pm 0.05 \\ 0.02 \pm 0.02 \end{cases}$ [40, 41]
$NH_3^+ + e^-$	$\rightarrow \begin{cases} NH_2 + H \\ \begin{cases} NH + H_2 \\ NH + 2\,H \end{cases} \\ \begin{cases} N + H_2 + H \\ N + 3\,H \end{cases} \end{cases}$	3.1×10^{-7} [13]	2 [this work]	0.5 – 1.5[this work]	-	0-1 [this work]
$NH_4^+ + e^-$	$\rightarrow NH_3 + H$	$9 - 15 \times 10^{-7}$ [1, 15, 42–44]	-	0.75 [1, 15, 43, 44]	0.2 [1, 15, 43, 44]	0.85 ± 0.04 [27, 40, 44, 45]
	$\rightarrow NH_2 + H_2$					0.2 ± 0.02 [27, 40, 44, 45]
	$\rightarrow NH_2 + 2H$					0.13 ± 0.01 [27, 40, 44, 45]
	$\rightarrow NH + H + H_2$					0.00 ± 0.01 [27, 40, 44, 45]
	$\rightarrow N + 2H_2$					0.00 ± 0.01 [27, 40, 44, 45]
$N_2^+ + e^-$	$\rightarrow (^4S)N + (^2D)N$	2.2×10^{-7} [46–53]	1.25 [46–53]	0.35 [46, 47, 49, 50, 53]	0.15 [46, 47, 49, 50, 53]	0.42 ± 0.10 [53, 54]
	$\rightarrow (^4S)N + (^2P)N$					0.09 ± 0.09 [53, 54]
	$\rightarrow (^2D)N + (^2D)N$					0.49 ± 0.10 [53, 54]
$N_2H^+ + e^-$	$\rightarrow N_2 + H$	2×10^{-7} [1, 15, 18, 55–60]	1.5 [1, 15, 18, 55–60]	0.5 [55, 58–60]	0.5 [55, 58–60]	0.95-1 [18, 23, 61]

Table 1: DR database *cont'd*

	reaction	$\alpha_0(cm^3.s^{-1})$	$F_{\alpha_0} = 1 + \frac{u(\alpha_0)}{\alpha_0}$	β	$\frac{u(\beta)}{\beta}$	b
	$\rightarrow$ NH + N					0-0.05 [18, 23, 61]
$CN^+ + e^-$	$\rightarrow$ (^4S)N + (^3P)C	3.4×10^{-7} [62]	1.16 [62]	0.55 [27, 62]	1 [this work]	$\leq$ 0.018 [62]
	$\rightarrow$ (^4S)N + (^1D)C					0.038 $\pm$ 0.028 [62]
	$\rightarrow$ $\begin{cases} (^2D)\text{N} + (^3P)\text{C} \\ (^4S)\text{N} + (^1S)\text{C} \end{cases}$					0.142 $\pm$ 0.014 [62]
	$\rightarrow$ $\begin{cases} (^2P)\text{N} + (^3P)\text{C} \\ (^2D)\text{N} + (^1D)\text{C} \end{cases}$					0.561 $\pm$ 0.026 [62]
	$\rightarrow$ $\begin{cases} (^2P)\text{N} + (^1D)\text{C} \\ (^2D)\text{N} + (^1S)\text{C} \end{cases}$					0.255 $\pm$ 0.014 [62]
	$\rightarrow$ (^2P)N + (^1S)C					$\leq$ 0.014 [62]
$HCN^+ + e^-$	$\rightarrow$ CN + H	2.5×10^{-6} [63]	2 [this work]	1 [63]	0.02 [63, 64]	-
$HNC^+ + e^-$	$\rightarrow$ CN + H	1.3×10^{-7} [63, 64]	1.7 [63, 64]	0.98 [63, 64]	0.02 [63, 64]	-
$HCNH^+ + e^-$	$\rightarrow$ HCN + H	3.2×10^{-7} [1, 65–67]	1.25 [1, 65–67]	0.65 $-$ 1.38 [65, 67]	-	0.26-0.41 [65, 68, 69]
	$\rightarrow$ HNC + H					0.29-0.39 65, 68, 69
	$\rightarrow$ $CN + H_2$					0 $\pm$ 0.017 [65]
	$\rightarrow$ CN + 2H					0.325 $\pm$ 0.032 [65]
$CH_2NH_2^+ + e^-$	$\rightarrow$ $\begin{cases} CH_3N + H \\ \begin{cases} {}^1CH_2 + NH_2 \\ {}^3CH_2 + NH_2 \end{cases} \\ \begin{cases} HCN + H_2 + H \\ HNC + H_2 + H \end{cases} \\ CN + 2\,H_2 \end{cases}$	$[0.5 - 3] \times 10^{-6}$ [this work]	-	0.5 $-$ 1.5 [this work]	-	$[0 - 1]$ [this work]
$CH_3NH_3^+ + e^-$	$\rightarrow$ unknown	14.0×10^{-7} [1]	2 [this work]	0.5 $-$ 1.5[this work]	-	-

Table 1: DR database *cont'd*

reaction	$\alpha_0(cm^3.s^{-1})$	$F_{\alpha_0} = 1 + \frac{u(\alpha_0)}{\alpha_0}$	β	$\frac{u(\beta)}{\beta}$	b
$CH_3CNH^+ + e^-$ → *a* { $CH_3CN + H$; { $C_2H_2N + H_2$; $C_2H_2N + 2\,H$ }; $C_2HN + H_2 + H$ } *b* $C_2N + 2\,H_2$	3.3×10^{-7} [1, 15, 51, 66, 67]	1.15 [66, 67]	1.03 [67]	1 [this work]	0.65 ± 0.03, a ∈ [0.25,1], b ∈ [0,0.25] [4]
→ *c* { $C_2H_4 + N$; $C_2H_2 + NH_2$; $C_2H_2 + NH + H$; $C_2H_2 + N + H_2$; $C_2H + NH_3$; $C_2H + NH + H_2$ } *d* { *e* { { $HCN + CH_3$; $HNC + CH_3$ }; { { $HCN +^1 CH_2 + H$; $HCN +^3 CH_2 + H$ }; { $HNC +^1 CH_2 + H$; $HNC +^3 CH_2 + H$ } }; { $HCN + CH + H_2$; $HNC + CH + H_2$ } } $CN + CH_3 + H$; *f* { $CH_3N + CH$; { $CH_2N +^1 CH_2$; $CH_2N +^3 CH_2$ }; $CN + CH_4$; { $CN +^1 CH_2 + H_2$; $CN +^3 CH_2 + H_2$ } } }					0.35 ± 0.03, $d \geq c$, $e \geq f$ [4]
$C_2N_2^+ + e^-$ → $2\,CN$	$0.5 - 3 \times 10^{-6}$ [this work]	-	0.5 – 1.5[this work]	-	- [70]
$C_3N^+ + e^-$ → $CN + C_2$	$0.5 - 3 \times 10^{-6}$ [this work]	-	0.5 – 1.5[this work]	-	- [13]
$CHCCN^+ + e^-$ → $C_3N + H$	$0.5 - 3 \times 10^{-6}$ [this work]	-	0.5 – 1.5[this work]	-	0.44 ± 0.04 [71]

Table 1: DR database *cont'd*

reaction	$\alpha_0(cm^3.s^{-1})$	$F_{\alpha_0} = 1 + \frac{u(\alpha_0)}{\alpha_0}$	β	$\frac{u(\beta)}{\beta}$	b
$\rightarrow \begin{cases} C_2H + CN \\ C_2 + H + CN \\ \begin{cases} HCN + C_2 \\ HNC + C_2 \end{cases} \end{cases}$					0.48 ± 0.05 [71]
$\rightarrow H + C + C_2N$					0.04 ± 0.02 [71]
$\rightarrow \begin{cases} C_2N + CH \\ N + C_3H \end{cases}$					0.02 ± 0.01 [71]
$\rightarrow HC_2N + C$					0.02 ± 0.01 [71]
$\rightarrow NH + C_3$					0.00 ± 0.01 [71]
$CHCCNH^+ + e^-$ $\rightarrow \begin{cases} \begin{cases} a \begin{cases} HC_3N + H \\ C_3NH + H \end{cases} \\ b \begin{cases} C_2NCH + H \\ HC_2NC + H \end{cases} \end{cases} \\ C_3N + H_2 \end{cases}$	$0.5 - 3 \times 10^{-6}$ [this work]	-	0.5 – 1.5[this work]	-	0.52 ± 0.05, $a \geq b$ [71, 72]
$\rightarrow \begin{cases} \begin{cases} HCN + C_2H \\ HNC + C_2H \end{cases} \\ CN + C_2H_2 \end{cases}$					0.48 ± 0.05 [71, 72]
$CH_2CHCNH^+ + e^-$ $\rightarrow \begin{cases} C_3H_3N + H \\ \begin{cases} C_3H_2N + H_2 \\ C_3H_2N + 2\,H \end{cases} \\ C_3HN + H + H_2 \\ \begin{cases} C_3N + 2\,H_2 \\ C_3N + 2\,H + H_2 \end{cases} \end{cases}$	1.76×10^{-6} [5]	1.17 [5]	0.80 [5]	0.025 [5]	0.50 ± 0.04 [5]

Table 1: DR database *cont'd*

reaction	$\alpha_0(cm^3.s^{-1})$	$F_{\alpha_0} = 1 + \frac{u(\alpha_0)}{\alpha_0}$	β	$\frac{u(\beta)}{\beta}$	b
$\rightarrow \begin{cases} CNH_3 + C_2H \\ CNH_2 + C_2H_2 \\ \begin{cases} HCN + C_2H_3 \\ HNC + C_2H_3 \end{cases} \\ \begin{cases} HCN + C_2H_2 + H \\ HNC + C_2H_2 + H \end{cases} \\ \begin{cases} HCN + C_2H + H_2 \\ HNC + C_2H + H_2 \end{cases} \\ CN + C_2H_4 \\ CN + C_2H_2 + H_2 \end{cases}$					0.49 ± 0.04 [5]
$\rightarrow \begin{cases} C_2H_3N + CH \\ \begin{cases} C_2H_2N +^1 CH_2 \\ C_2H_2N +^3 CH_2 \end{cases} \\ C_2HN + CH_3 \\ C_2N + CH_4 \\ C_2N + CH_3 + H \\ NH_3 + C_3H \\ NH_2 + C_3H_2 \\ NH + C_3H_3 \\ N + C_3H_4 \end{cases}$					0.01 ± 0.01 [5]
$C_2H_5CNH^+ + e^-$ → unknown	4.6×10^{-7} [66, 67]	1.15 [66, 67]	0.81 [67]	1 [this work]	-
$H_2O^+ + e^-$ → OH + H	3.34×10^{-7} [1, 15, 73, 74]	1.30 [1, 15, 73, 74]	0.77 [1, 15]	0.05 [1, 15]	0.25 ± 0.1 [17, 73–75]
→ O + H_2					0.10 ± 0.06 [17, 73–75]
→ O + 2 H					0.65 ± 0.1 [17, 73–75]
$H_3O^+ + e^-$ → OH + 2 H	8×10^{-7} [1, 20, 76, 77]	1.5 [1, 20, 76, 77]	0.9 [76, 78]	0.12 [76, 78]	0.60 ± 0.15 [17, 77–80]
→ H_2O + H					0.25 ± 0.05 [17, 77–80]
→ OH + H_2					0.14 ± 0.05 [17, 77–80]
→ O + H_2 + H					0.01 ± 0.05 [17, 77–80]

Table 1: DR database *cont'd*

reaction	$\alpha_0(cm^3.s^{-1})$	$F_{\alpha_0} = 1 + \frac{u(\alpha_0)}{\alpha_0}$	β	$\frac{u(\beta)}{\beta}$	b
$CO^+ + e^-$					
$\rightarrow C + O$	2.0×10^{-7} [51, 81, 82]	1.5 [51, 81, 82]	0.55 [81]	1 [this work]	-
$HCO^+ + e^-$					
$\rightarrow CO + H$	2.1×10^{-7} [1, 13, 15, 18, 20, 55, 59, 83–85]	1.41 [1, 13, 15, 18, 20, 55, 59, 83–85]	0.69 [1, 13, 15, 27, 55, 59]	0.45 [1, 13, 15, 27, 55, 59]	0.92 ± 0.03 [45, 59]
$\rightarrow C + OH$					0.07 ± 0.02 [45, 59]
$\rightarrow O + CH$					0.01 ± 0.01 [45, 59]
$CH_2OH^+ + e^-$					
$\rightarrow H_2O + CH$	7×10^{-7} [86]	2 [this work]	0.78 [86]	1 [this work]	0.022 ± 0.022 [86]
$\rightarrow CH_2 + OH$					0.055 ± 0.055 [86]
$\rightarrow$ HCOH + H					
$\rightarrow$ HCO + H_2					
$\rightarrow$ HCO + 2 H					0.923 ± 0.1 [86]
$\rightarrow$ CO + H_2 + H					
$\rightarrow$ CO + 3 H					
$NO^+ + e^-$					
$\rightarrow (^4S)N + (^3P)O$	4×10^{-7} [1, 13, 17, 48, 87–89]	1.50 [1, 13, 17, 48, 87–89]	0.8 [1, 13, 89]	0.5 [1, 13, 89]	0.85 ± 0.06 [17, 90]
$\rightarrow (^4S)N + (^1D)O$					0.15 ± 0.06 [17]
$\rightarrow (^2D)N + (^3D)O$					
$OH^+ + e^-$					
$\rightarrow O + H$	3.75×10^{-8} [1, 13, 15, 91]	2 [this work]	0.5 [1, 13, 15, 91]	1 [this work]	-

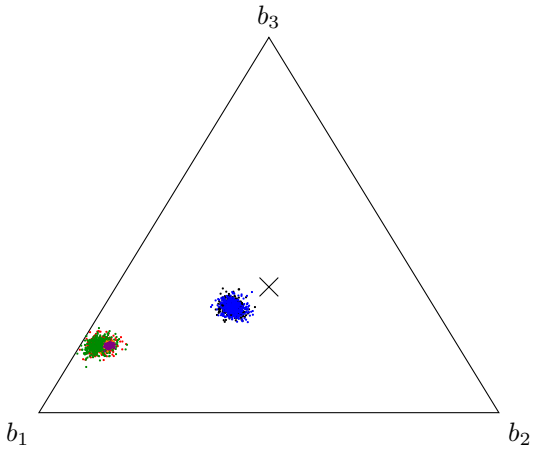

Figure 2: A normalization to unity or changing only the maximal value has no consequences over the sampled space, as this modification is always smaller than the measurements' uncertainties. Black dots: C_4H^+ DR branching ratios normalized to unity; blue dots: C_4H^+ DR branching ratios with a recalculated maximal value; red dots: $C_4H_2^+$ DR branching ratios normalized to unity; green dots: $C_4H_2^+$ DR branching ratios with a recalculated maximal value; orange dots: $C_4H_3^+$ DR branching ratios normalized to unity; violet dots: $C_4H_3^+$ DR branching ratios with a recalculated maximal value.

Notes

- Sometimes the sum of the branching ratios found in the literature does not sum to one. In this case, it has been chosen to modify the maximal value. This change is specified when necessary, the reported measured value is given in parenthesis. This choice rather than renormalizing the whole set is actually of no consequence. Indeed, the differences implied by either a renormalization or the change in the maximal value are by the measurements' uncertainties. (see Fig. 2 for a three dimensions example).

- $HCNH^+$: The available data are for the ratio and the sum of the two species HNC and HCN. The ratio is characterized by Ishii et al. [69] ($0.77 \leq \frac{[HCN]}{[HNC]} \leq 1.32$) and the sum by Semaniak et al. [65] ($[HCN] + [HNC] = 0.675 \pm 0.016$). The values given in the database have been figured out from a Monte Carlo propagation with the former equations, they are in agreement with Hickman et al. [68] calculations, no further spreading of the branching ratios was necessary.

- l,c–$C_3H_3^+$: the measurements of the $C_3H_3^+$ dissociative recombination rate and branching ratios are difficult to translate into a database. McLain et al. [32] give two different global rate constants for the l and c species, but the branching ratios only for the global form $C_3H_3^+$ of the species. Angelova et al. [30] give the branching ratios as follows:
  We find that the most probable channel for the recombination of $C_3H_3^+$ is the C_3 channel accounting for 90.7% of the total. This channel corresponds to the loss of a single hydrogen atom or to the loss of a H_2 molecule from the cyclic ion. The linear ion, if recombining, can also lose two separate H atoms. The C_2 + C channel is not negligible, and accounts either for a unique C–C bound break in the linear ion, or for ring opening in the cyclic ion. In this case, two C–C bounds must be broken, or considerable rearrangement must occur prior to splitting.
  Florescu-Mitchell and Mitchell [1] translate into actual channels with

$$C_3H_3^+ + e^- \begin{cases} \rightarrow \begin{cases} C_3H_2 + H \\ C_3H + H_2 \\ C_3H + 2H \end{cases} \\ \rightarrow \begin{cases} C_2H + CH_2 \\ C_2H_2 + CH \\ C_2H_2 + C + H \end{cases} \end{cases}$$

  We translated it with each isomer giving all the channels, even though this is not what is actually happening.

- There is an actual controverse over CH_5^+, indeed Molek et al. [23] unsing a Flowing Afterglow Electron Ionizer (FAEI) found totally different results than the previous storage ring (SR) experiment [21]:

		Molek et al. [23] (FAEI)	Semaniak et al. [21] (SR CRYRING)
$CH_5^+ + e^-$	$\rightarrow CH_4 + H$	95±5%	4.9±1.3%
	$\rightarrow CH_3 + H_2$	≤ 8%	4.8±0.2%
	$\rightarrow CH_3 + 2H$		69.8±0.8%
	$\rightarrow CH_2 + H + H_2$	≤ 1%	17.2±1.6%
	$\rightarrow CH + H_2 + H_2$	≤ 1%	3.3±1.1%

They explain the discrepancies by the fact that CH_4 have a stated trend to form CH_3 by DR, and thus their produced CH_4 is consumed by the electrons. The CRYRING values for the branching ratios are taken at a null center-of-mass energy.
The SR scheme was implemented in the present model.

- C_2H^+, $C_2H_2^+$ and $C_2H_3^+$: Florescu-Mitchell and Mitchell [1], Stockholm University [15] take their rate constant and temperature dependencies from Mul and McGowan [92]. It is to be noted that the α_0 value reported in Stockholm University [15] is the 100 K rate constant value in Mul and McGowan [92] and that the proposed parameters in Florescu-Mitchell and Mitchell [1] do not yield the 100 K value of Mul and McGowan [92].

- CH_4^+, NH_3^+: the branching ratios are the combinatorics with a limitation to a three-body breakup. Indeed, three-body breakups are exceptionnal at those collision energies and four-body breakups have been observed at high temperatures. Novotnỳ et al. [93] give thresholds of 3.3 and 5.3 eV for the four-body dissociation channels of the DR of D_3O^+, which corresponds to electron temperatures of 38,295 K and 61,504 K. These temperatures are largely too high to be considered for this database. No thermodynamics considerations are done, thus a total uncertainty is stated.

- $C_2H_5^+$, $CH_3CNH_3^+$, $CHCCN^+$, $CHCCNH^+$: the neutral products and branches are taken as analogous to the deuterated species. Geppert et al. [28] measured the branching ratios for the DR of $C_2D_5^+$, Vigren et al. [4] for the DR of CD_3CND^+, Geppert et al. [71] for $DCCCN^+$ and $DCCCND^+$, which complete Osamura et al. [72] calculation for the DR of $CHCCNH^+$. Larsson et al. [34] discuss the comparison of $C_3H_7^+$ and $C_3D_7^+$ dissociative recombination branching ratios. The values of the branching ratios are stated as totally uncertain.

- H_3^+: The values of the rate constant at 300 K for the dissociative recombination of H_3^+ was a very challenging issue, as the measurements would be discrepant up to a factor of 10^5. In Larsson et al. [8] paper, they give a review of the "H_3^+–saga", and the most probable value appears to be the calculated value of Kokoouline and Greene [6, 7] of 7.2×10^{-8} $cm^{-3}.s^{-1}$ at a 15% precision.

- $C_3H_7^+$: The value of Ehlerding et al. [2] is considered as certainly too high by Larsson et al. [34], a unique procedure of two-step normalization being the potential cause of this biais. Nonetheless, considering this value with its uncertainty ($1.6 \times 10^{-6} \pm 0.35$ (1σ level) in $cm^{-3}.s^{-1}$) in regard of Lehfaoui et al. [19] previous value of 8.7×10^{-7} $cm^{-3}.s^{-1}$, given with a 30% uncertainty (no equivalence in σ given). Thus with the hypothesis that the uncertainty of Lehfaoui et al. [19] is at a 2σ level, we found an interval of [4.785–29.5] at a 3σ level in 10^{-7} $cm^{-3}.s^{-1}$ units for the elicitation, which justify the use of the interval [5,30] in 10^{-7} $cm^{-3}.s^{-1}$ as the maximum interval in case of no information.

- $C_6H_6^+$ is the benzene isomer only.

- N^+ and C^+: Nahar and Pradhan [12] calculated the rate constant over a range of temperature, we performed a fit, wich we found to be corresponding to Woodall et al. [13] values from the same fit. The RMS errors we found on our fit are lower than the uncertainties reported in Woodall et al. [13], thus we report here the biggest uncertainty values.

- For unknown α_0 of small molecules - typically small nitriles - it was found more reasonnable to establish an upper limit to 10^{-6} $cm^{-3}.s^{-1}$ rather than the high value of 3×10^{-6} $cm^{-3}.s^{-1}$, suitable for heavy hydrocarbons (see Adams et al. [27], Adams and Babcock [60], Tab. 1 and Fig. 8 resp.), and a lower bound of 5×10^{-8} $cm^{-3}.s^{-1}$

- CNC^+, NH_2^+, $C_2N_2^+$: the trend for the rate constant at 300 K to increase has been observed by Adams et al. [27], Adams and Babcock [60] for hydrocarbons, but as far as small molecules are concerned, the rate constants at 300 K are either smaller or in the 10^{-7} order of magnitude in $cm^{-3}.s^{-1}$. We thus chose an interval of $0.5 - 10 \times 10^{-7}$ as the interval of maximum amplitude for small nitriles for which the rate constant at 300 K is unknown, see above point.

- N_2H^+: Amano [55] provide measurements at 110, 210 and 273 K. A bayesian fit of the form $\alpha(T_e) = \alpha_0.\left(\frac{T_e}{300}\right)^{-n}$ provides $\alpha_0 = 6.6 \pm 0.4 \times 10^{-7}$ cm^{-3}.s^{-1} and $n = 0.75 \pm 1$ (within the [0.5,1.5] bounds). Adams and Babcock [60], Tab. 2 perform the same calculations and give a similar results (7.1×10^{-7} cm^{-3}.s^{-1}). Yet those measurements are made for vibrationnally excited molecules, and as they are very discrepant with other measures, giving a value around 2×10^{-7} cm^{-3}.s^{-1}, they were not taken into account for this elicitation.

  Geppert et al. [57, 59] give from CRYRING results a branching ratio of *circa* 2/3 for the NH + H channels. However, Molek et al. [23, 61] suspect the parasitic reaction $^{15}N^{14}N + e^- \rightarrow {}^{15}N + {}^{14}N$ and a detection of ^{15}N to be the reason for a measurement of so high a value for the NH channel.

- HCN^+/HNC^+: The notation CHN^+ in Sheehan et al. [64] denotes an unknown mixture of the two isomers HCN^+ and HNC^+. Sheehan et al. [64] measured a rate constant of the form $\alpha(T_e) = 3.9 \times 10^{-7}\left(\frac{T_e}{300}\right)^{-0.96}$ for CHN^+ DR, and a rate constant of the form $\alpha(T_e) = 1.82 \times 10^{-7}\left(\frac{T_e}{300}\right)^{-0.96}$ for the HNC^+ isomer DR. Talbi et al. [63] calculated rate constants as $\alpha_{HCN^+}(T_e) = 2.5 \times 10^{-6}\left(\frac{T_e}{300}\right)^{-1}$ and $\alpha_{HNC^+}(T_e) = 9 \times 10^{-8}\left(\frac{T_e}{300}\right)^{-1}$. Talbi et al. [63] and Sheehan et al. [64] have a factor 2 between the measured and calculated values of the DR of HNC^+, thus we elicited HCN^+ with the calculated value and a 100% uncertainty.

- $C_2N_2^+$, $C_2HN_2^+$: Woodall et al. [13] give estimations of the rate constant and branching ratios, we thus considered the given channels and stated a total uncertainties over the values of the rate constants, the branching ratios and the possible isomers (HNC and HCN for $C_2HN_2^+$ DR).

- CN^+: the different isomers of the carbon are given, even though the differenciation is not made in the model. We kept the different isomers because of the nested pattern which do not allow to put together the channels with common nitrogen.

- H_3O^+: Williams et al. [94] provide branching ratios that are in contradiction with the other measurements: they were not taken into account.

- CH_2OH^+: we have access only to Hamberg et al. [86] abstract, and no thermodynamics data have been found. Thus for the conservation of the C-O bound, it is the combinatorics up to all the possibilities. If the CO + 3 H channel is not thermodynamically possible, it should not be of great consequences: in Vuitton et al. [95] mass spectrum assignation, CH_2OH^+ does not appear, and in a steady state of our model, its density is about 0.25 ± 0.2 cm^{-3} at 1100 km (neutral species densities taken from **?**]).

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