Dissociative recombination

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Contents

1 Update to perform !!!

$N_2^+, C_3H^+, C_3H_6^+, C_3H_8^+, C_4H^+, C_4H_2^+, C_4H_6^+, C_4H_8^+$ Beware of H repartition, not balanced in $C_3H_5^+, C_3H_6^+, C_3H_8^+$

2 Litterature review : what is it and how is it done ?

2.1 The Book

Dissociative Recombinations of Molecular Ions of Mats Larsson and Ann E. Orel. Gives the very interesting database http://www.physto.se/DRdatabase. I strongly suggest a view of this site. I'll update my database with it (spotted CH_4^+ or branching ratio of big hydrocarbon ions for instance).

> ➤ pg. 24, 1st §: " There is a factor of 2 error in this paper, which means that cross-section measured between 1977 and 1985 using MEIBE are a factor of 2 too large (Mitchell 1990a)."

> ➤ pg. 27, 2nd §: "[...] list of the advantages and disadvantages of the merged-beam technique.
> > Advantages : (i) very wide energy range; (ii) high energy resolution; (iii) absolute cross-section measured; (iv) product branching ratios can be measured; (v) long interaction path gives high signal count rate.
> > Disadvantages : (i) up to now reactant-ion excitation states have not been well determined; (ii) in the present form, limited to molecular weights less than 32."

2.2 Litt. review

The original vibrationnal state is difficult to control, yet the dissociative recombination is very sensitive to the initial vibrationnal state of the ion species. It makes the discrimination between direct or indirect mechanism. Direct is going from reactants to products directly, indirect suppose to pass through a high energetic Rydberg state, the indirect mechanism is experimentally seen by a resonance. That's why in plasma you forget it (too hot), and there

are big problems with the merged-beam method, even when buffer gaz are used (Ne or He) [1]. Then the heavy-ion storage-ring technique is well adapeted because one can store the ion species long enough to vibrationnaly relax [2], which is interesting for low temperature measurements. Indeed it's possible to have cold electrons, which gives thermalized electrons which are expected in Titan's ionosphere for example. The best experimental measures are then expected with the latest method [2]. For knowing what a storage ring is, specially CRYRING, see Larsson [3].

Accepted that, for the direct mechanism :

$$\alpha_e(T_e) = \alpha_{e0}(\frac{T_e}{300})^{-0.5}$$

with α_{e0} rate coefficient at 300 K and T_e the electron temperature. For indirect mechanism

$$\alpha_e(T_e) \text{ vary as } \alpha_{e0}(\frac{T}{300})^{-1.5}$$

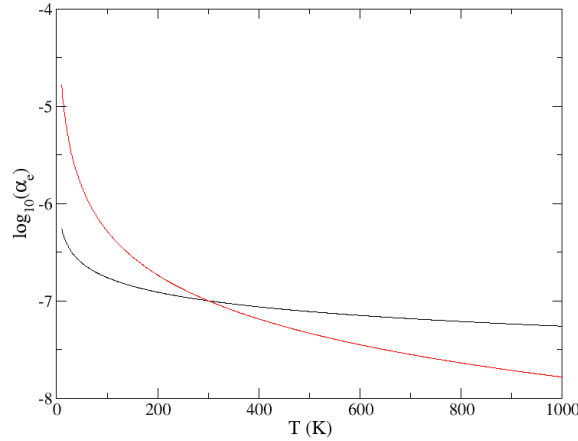with T the electron and ion temperature [4], which so suppose the electrons to be thermalized (see Fig. 1).

Figure 1: Direct (black) and indirect (red) mechanisms, α_{e0} is taken arbitrary equal to 1.10^{-7} $cm^3.s^{-1}$, T is the electron and ions temperature as the electrons are thermalized

Most of the time, it's a mix of the two, then it explains the discrepancies on the power. This could explain the big differences found in the litterature for rate constants. In fact, I clearly wonder if we should not split the pdfs into two sub-pdfs, one indirect and one direct [5]. Mouais bof, as it depends strongly of the species... bof, bof, the splitting is in the power, we have no experimental access to data concerning only one of these two separated mechanisms. And I don't even think about the possible tunneling [I don't remember the ref, somewhere in the articles at the end]... Maybe one day I'll try and fit their $\sigma(E_{cm})$ with this type of function (meaning the sum of the two mechanisms)... As indirect mechanism may need to get into an excited state, which is not necessarily easy (HNC for instance), there's quite a trend for ground states to undergo direct mechanism and excited states indirect mechanism. The process of DR needs a crossing between the electronic curves, and it is not simple. That problem seems to be on the way for three-boby molecules, it could explain the H_3^+ issue.

I'd like to highlight Adams et al. [6], this one's good and should be given a peculiar attention. It's a good briefing of what's done, what's known, where we are.

One except : "Unlike ion molecule reactions, no full compilations of rate coefficient, α_e, have been produced for electron-ion dissociative recombination. However, several reviews have been written, each of which contains a proportion of the data. This review will continue in that vein, especially since complete list are being compiled." The refs are not given (yet), the compiling is known from Johnsen, private communication and Huestis 2005. Pg 16, on $C_2H_3^+$, error, a 6 for 0.6 % for the $CH_3 + C$ products channel.

2.3 Coding

Representation in *mc_ion_unc_tot* :

$$\alpha_e = \alpha_{e0} \times (\frac{T_{ref}}{T_e})^{pwr} \times br$$

with T_e the electron temperature, given in file electron_temp.*extension(:ld)*, Marek values, T_{ref} given in recomp*.dat, 300 K, pwr given in recomp*.dat (see below) and br also (see also below). *my_ions* calculates T_e (same hypothesys/fashion) and uses partial constant rates instead of global times branching ratios.

3 Obtaining the data

3.1 The rate constant

What's actually measured is σ, the relation between σ and α_e is :

$$\alpha_e(T_e) = \frac{8\pi m_e}{(2\pi m_e k T_e)^{\frac{3}{2}}} \int_0^\infty E_{cm}\sigma(E_{cm})e^{-\frac{E_{cm}}{kT_e}} \, dE_{cm}$$

with :

- $\succ$ T_e : electron temperature
- $\succ$ k : Boltzmann constant
- $\succ$ m_e : electron mass
- $\succ$ E_{cm} : center of mass energie (between the ion and the electron),

so a calculation is needed to extract α_{e0} (i.e. α_e at 300 K) and $\alpha_e(T_e)$ at all T_e wanted and then a fit is done to get the precedent given shape. So it's not a direct measurement, but a fit. I present in the next section some calculations, but keep in mind that gaussian process are more efficient.

3.2 The branching ratios

When the final branches are not explicitly known, some theoretical investigations are due. For instance, $C_4H_9^+$ which is given in Mitchell et al. [7], uses the results of Smith and Radom [8] for the final branching ratios. And this work is about heavy *ab initio* calculations. For some species, nothing is given as a reason for the chosen final branches. This is the case for $C_3H_7^+$ in Ehlerding et al. [32].

3.3 Computation

Sometimes papers don't give the rate constant, they stop at the cross section. So I computed the equation.

3.3.1 NH_4^+

I took Öjekull et al. [9] for reference. The measurements of σ stop at 10^{-3} eV, so there's a need to extrapolate to lower energies (as it can be easily proved, α_e depends more strongly of the σ at low energies than high). Two limiting cases, σ is constant below 10^{-3} eV or the energy dependance is still the same (as an activation barrier is expected [10]).

I started with their fit of σ, which is :

$$10^{-3} \leq E_{cm} < 0.124 \, eV \quad \sigma(E_{cm}) = 10^{-14.84\pm0.02} \times E_{cm}^{-1.10\pm0.01}$$

$$0.124 \leq E_{cm} < 0.341 \, eV \quad \sigma(E_{cm}) = 10^{-15.34\pm0.02} \times E_{cm}^{-1.66\pm0.03}$$

$$0.341 \leq E_{cm} < 1.0 \, eV \quad \sigma(E_{cm}) = 10^{-16.19\pm0.05} \times E_{cm}^{-3.47\pm0.20}$$

The rectangle approximation biais, beware on how you count

> This paragraph about the rectangle approximation biais is to show the errors that can happen just because the calculation means is bad.

I added a strong correlation between those two uncertain parameters (justification by the fact that their uncertainties are clearly too small for a correlation not to be there...). One must extrapolate below 10^{-3}eV so as to have a good estimation of the rate constant. As at 0 eV, $\sigma \mapsto \infty$ (0 power something negative), one needs to define a lower calculation bound. The curves of Fig. 2 were calculated with a lower bound of 10^{-10}eV.

This integration method is very sensitive to the used lower bound, as it is shown in Fig. 3, and therefore must absolutely not be used.
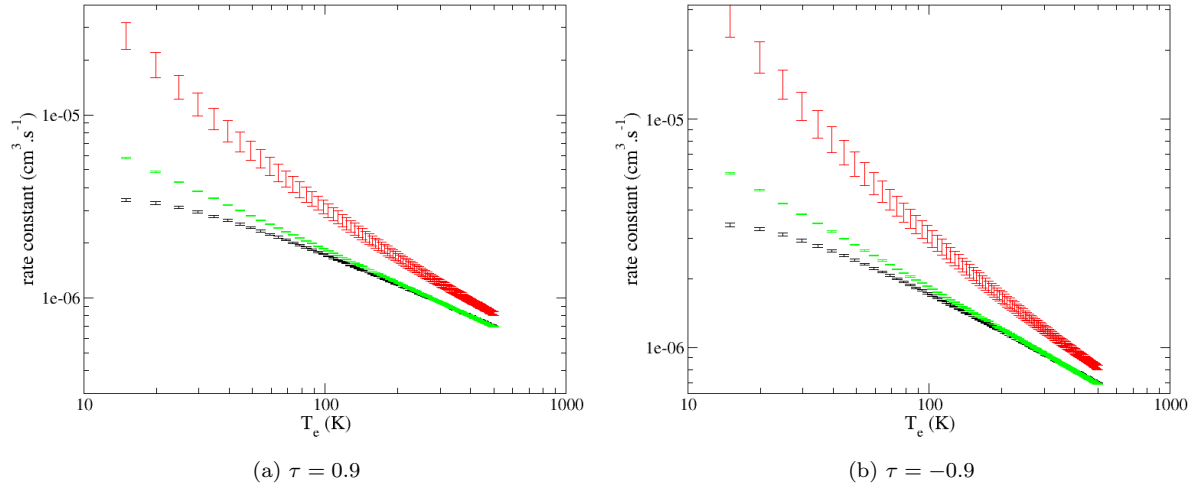
(a) $\tau = 0.9$

(b) $\tau = -0.9$

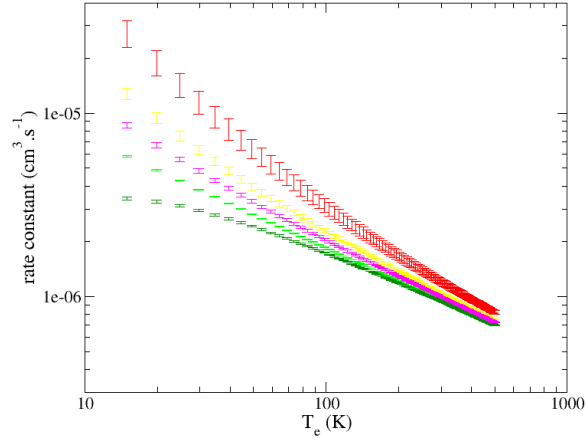Figure 2: Limiting cases : black, constant ; red, same energy dependancy ; green, their estimations.

Figure 3: Lower bound dependency. dark green : no extrapolation, black : constant (below dark green), green : them, red : 10^{-10}, yellow : 10^{-8}, blue : 10^{-5}, magenta : 10^{-4} eV
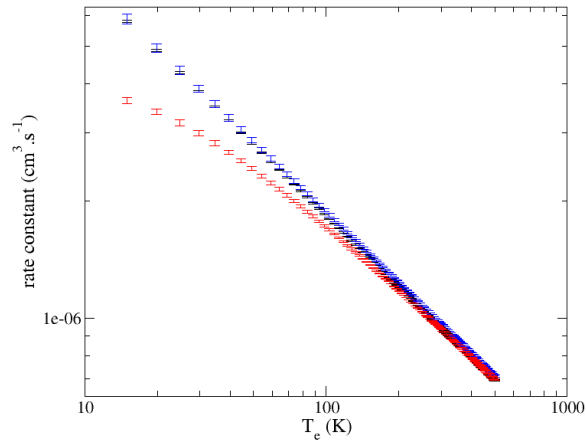

Figure 4: Rigorous integral calculation, black : their estimations, red : constant, blue : extrapolation

Better integration calculation technique   I changed the integral calculation[a]. The results are shown in Fig. 4

It seems they don't take into account the fact that uncertainty increases du to the lack of knowledge at low temperatures (as they seem to calculate only the extrapolated curve), so I would advise to increase a lot their uncertainties... Please note too that the uncertainty they give (and reported in the table below, used here as a standard deviation) is their 95% confidence intervalle, so my $1 - \sigma$ level is their $2 - \sigma$ level of description. At 300 K, they give :

$$\alpha_{e0} = 9.44 \pm 0.03 \, 10^{-7} \text{cm}^3.\text{s}^{-1} \quad 95\% \text{ confidence interval}$$

I find, using a $2 - \sigma$ standard deviation :

$$\alpha_{e0} = 9.44 \pm 0.03 \, 10^{-7} \text{cm}^3.\text{s}^{-1} \quad 66\% \text{ confidence interval}$$

so with a $2 - \sigma$ on input, I find 2 times their σ on output.

In brief : I validated my rate constant calculation, the mean of calculation is very important, and I think that they underestimate their uncertainties because they consider only the extrapolated case.

Lower Energies influence   It's very important to have measurements at the lowest possible energies. I recalculated the rate constant with DuBois et al. [11] values. They measured the cross-section down to 0.065 eV but didn't calculate the corresponding rate constant. They had the following fit for the cross section :

$$0.050 \leq E_{cm} \leq 0.3 \, \text{eV} \quad \sigma(E_{cm}) = 4.30 \, 10^{-16} \times E_{cm}^{-1.40}$$

$$0.3 < E_{cm} \quad \sigma(E_{cm}) = 3.73 \, 10^{-17} \times E_{cm}^{-3.43}$$

with a 60 % estimated uncertainty. I put a standard deviation of 6% of the value (for the coefficient and the power), I took the two same extreme cases. Fig. 5 shows that nothing is for granted, indeed, more precise measurements on the cross-section gives altogether different results over the rate constant.
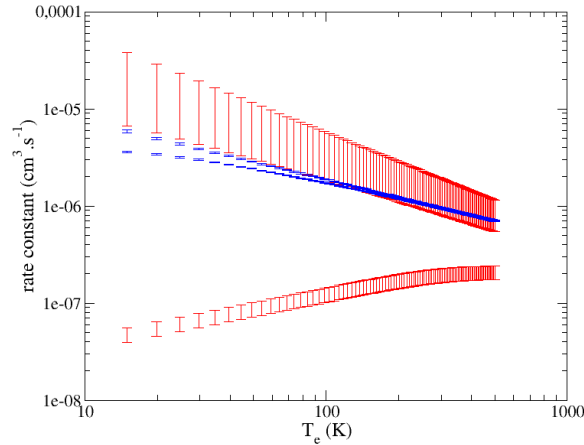

Figure 5: Comparison of two series of σ measurements. Blue : Öjekull et al. [9] ; red : DuBois et al. [11]. The limiting cases are represented.

3.3.2 $C_2H_3^+$

I've taken $C_2H_3^+$ to test a little bit further. From Kalhori et al. [12], I used a scanned sigma-curve.

Several remarks :

➤ Measurements from 10^{-6} to 10^{-1} eV $\Rightarrow$ about 10^{-2} to 10^2 K, ($k_B = 8.617 \, 10^{-5}$ eV.K^{-1}), the center-of-mass energy (measured one) is considered (in this work, so as to extrapolate on Titan) as the energy of the medium ($E_{cm} = E_e = E_{ion}$, which means $T_e = T_{ion} \Leftrightarrow$ the electrons are thermalized).

➤ I didn't take into account the uncertainties over the energies (0.5 meV at lowest energies, 3 meV at highest - they don't give a threshold to tell low enegies from high)

➤ They calculate the rate constant over the temperature range [50; 3000] K (how did they evaluate that interval ? It doesn't correspond at all to the range of temperature I evaluated.)

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[a]subroutine gauleg, between 0 and 10, nstep=1000, which gives an inferior limit of $1.44 \, 10^{-5}$ and an upper limit of 9.999999, I found the convergence (in number of steps - lower bound - and upper limit)

- ➤ The results they give over the rate constant is :

  - ⋈ At low temperatures, the power law is a $T^{-0.84}$ law, at high temperatures, it is a $T^{-1.38}$ power law, the change occurs between 700 and 1000 K, deduced from their Fig. 7.
  - ⋈ $\alpha_e(300\,\mathrm{K}) = \alpha_{e0} = 5 \times 10^{-7}\,\mathrm{cm^3.s^{-1}}$

- ➤ So their results should be $\alpha_e(T) = 5 \times 10^{-7} \times (\frac{T}{300})^{-p}$, $\begin{cases} p = 0.84\ if\ T \leq 850\,K \\ p = 1.38\ if\ T \geq 850\,K \end{cases}$

- ➤ I consider $T < 500$ K[b], so their $\alpha -$ curve is $\alpha_e(T) = 5 \times 10^{-7} \times (\frac{T}{300})^{-0.84}$

First fit, I use their fit   I fitted it with two lines (in log-log scale), the first (low energies) is the fit from xmgrace, the second (high energies) is a fit obtained on my appreciation with their power imposed. I had pretty good agreement with their figures. But the uncertainties seem to need to be a lot larger than expected.
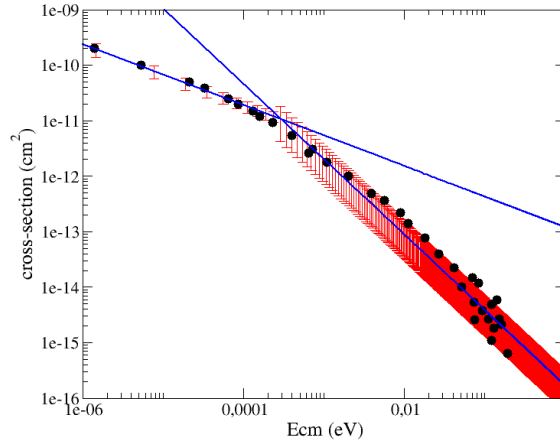

Figure 6: Black dots : scanned data, blue curves : fits, red : generated for the rate constant calculations

The fits have the form $\sigma(E_{cm}) = P_1 \times E_{cm}^{P_2}$. I took as fit parameters :

- ➤ lower energies fit :

  - ⋈ $P_1 = 1.2\,10^{-13}$
  - ⋈ $P_2 = -0.55$

- ➤ higher energies fit :

  - ⋈ $P_1 = 2.0\,10^{-16}$
  - ⋈ $P_2 = -1.36$

The first fit is given by xmgrace fit, the second adapted so as to have the power over the energy given in the paper. The uncertainties are given as 20 % at lower energies and then the scattering gives it. I took a 20 % uncertainty at a $1 - \sigma$ level for $P_1 -$ low parameter, and a 71 % $1 - \sigma$ level for $P_1 -$ high. An absolute uncertainty of 0.1 at a $1 - \sigma$ level for P_2 parameters (these ones I'm not sure how it's supposed to be handled in the paper) has been considered. The dispersion is gaussian. The rate constant is given in Fig. 7.
So I guess 1.2 for the uncertainties is not enough...

Second fit, I do it myself with the same expression   I redid the extrapolation, first one all or nothing method at a $1 - \sigma$ level (see Fig. 8), I coded in the Hercourt-Hessen form :

$$\sigma(E_{cm}) = 10^{P_1} \times E_{cm}^{-P_2}$$

I have three parts :

- ➤ $E_{cm} < 2\,10^{-4}$eV :

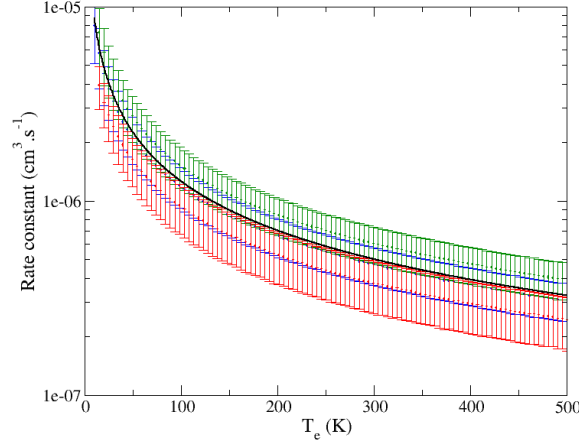[b] At 1100 km, the used electron temperature is 180 K

Figure 7: Generated rate constant (red), their results (black), from my database (blue), from Woodall et al. [13] (green). They don't give uncertainties over the calculated rate constant.

⋈ $P_1 = -13.22 \pm 1.5\,10^{-2}$, $1 - \sigma$ level

⋈ $P_2 = 0.610 \pm 3.4\,10^{-3}$, $1 - \sigma$ level

⋈ Kendall's tau = -0.75

≻ $2\,10^{-4} \leq E_{cm} < 2\,10^{-2}$ eV :

⋈ $P_1 = -14.89 \pm 1.5\,10^{-2}$, $1 - \sigma$ level

⋈ $P_2 = 1.05 \pm 1\,10^{-2}$, $1 - \sigma$ level

⋈ Kendall's tau = -0.85

≻ $2\,10^{-2} \leq E_{cm}$ (eV) :

⋈ $P_1 = -16.57 \pm 8\,10^{-2}$, $1 - \sigma$ level

⋈ $P_2 = 2.05 \pm 6\,10^{-2}$, $1 - \sigma$ level

⋈ Kendall's tau = -0.96

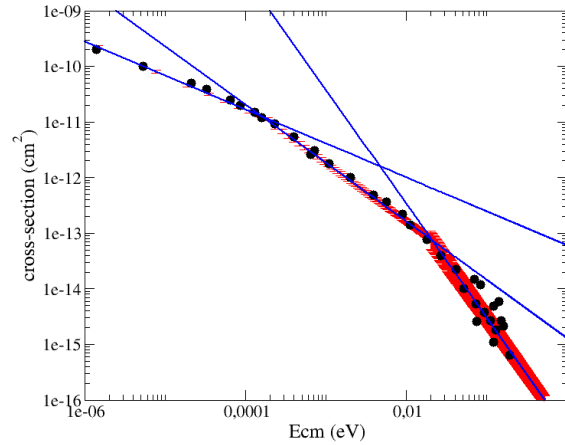For this fit I took 20 % error on each data point.

Figure 8: Interpolation of the cross-section. Hercourt-Hessen, all or nothing at a $1 - \sigma$ level.

It gives the rate constant depicted in Fig. 9 :

To obtain a fitted expression of α_e, another fit is needed. The Hercourt-Essen equation won't fit well the rate constant. I took then an equation of the Berthelot Hercourt-Essen (BHE) form :

$$\alpha_e = A \times T^P \times e^{D.k_B.T}$$
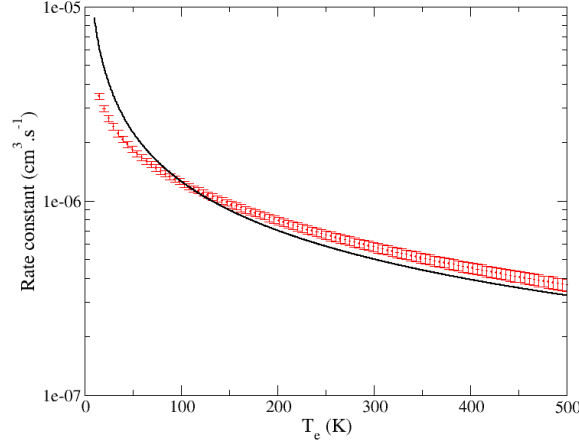
It works quite well. I have the following results Fig. 10:

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Figure 9: α_e obtained with a $1 - \sigma$ description level. Red : me ; black : them

➤ $\ln(A) = -11.27 \pm 3\,10^{-2}$

➤ $p = -0.48 \pm 1\,10^{-2}$

➤ $D.k_B = -1.0\,10^{-3} \pm 2\,10^{-4}\ K^{-1}$

➤ correlation matrix (Spearman) :
$$
\begin{array}{ccc}
ln(A) & p & D.k_B \\
1. & -0.9 & 0.4 \\
-0.9 & 1. & -0.7 \\
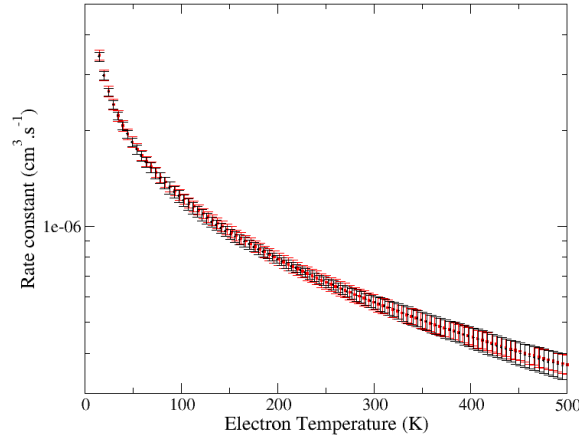0.4 & -0.7 & 1.
\end{array}
$$

Figure 10: Fitting the rate constant, red : target ; black : fit

Be really careful with this first fit. I did an all-or-nothing method, the threshold being $1 - \sigma$, it's just so I have an idea of how it's gonna look.

Then I fitted the cross-section with these expressions too, to have a better fit, and see how it plays over the rate constant.

Second fit, with another expression I used the BHE expression and Van't Hoff expression. The most complete equation (Van't Hoff) is :

$$\ln(\sigma) = p \times \ln(E_{cm}) + A - \frac{E_a}{E_{cm}} + D.E_{cm}$$

with :

➤ p : the power

➤ A : a factor (it's e^A with regard to the previous fit)
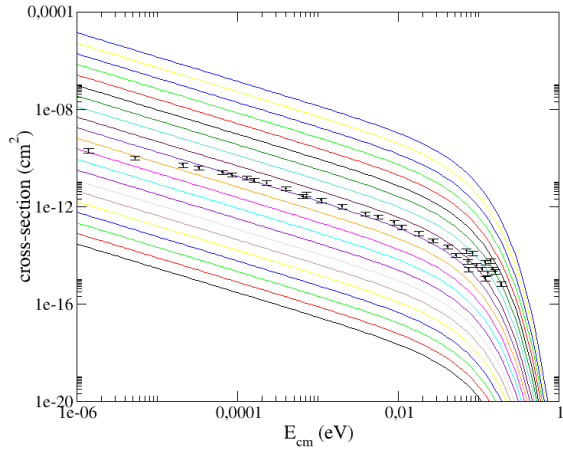
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> E_a = activation energy

> D = Berthelot

First I study the influence of each factor, the others being non-variant. I used :
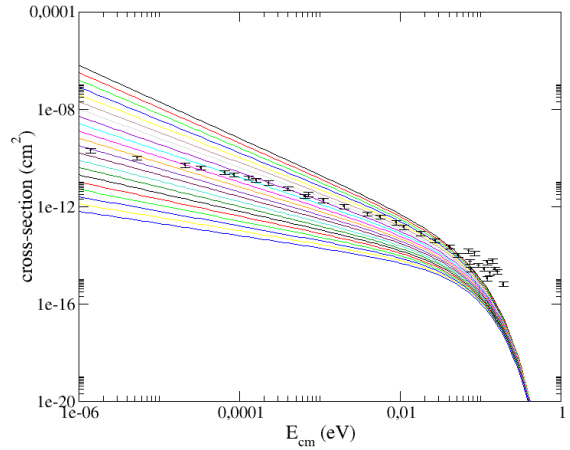
> A varying between -40 and -20, A=-30 when fixed

> p varying between -1.5 and -0.5, p=-1 when fixed

> E_a varying between -1.10^{-5} and 1.10^{-5} eV, $E_a = 0$ eV when fixed

> D varying between -40 and -20 eV^{-1}, D=-30 eV^{-1} when fixed

(a) A $\in$ [-40,-20], p=-1, $E_a = 0$ eV, D=-30 eV^{-1} (b) A=-30, p $\in$ [-1.5,0.5], $E_a = 0$ eV, D=-30 eV^{-1}
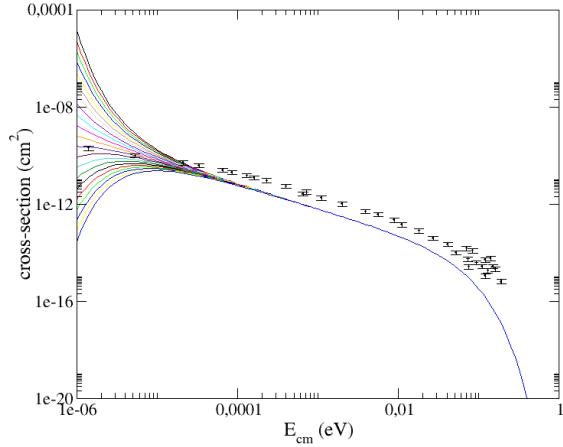
(c) A=-30, p=-1, $E_a \in [-1\,10^{-5}, 1\,10^{5}]$ eV, D=-30 eV^{-1} (d) A=-30, p=-1, $E_a = 0$ eV, D $\in$ [-40,-20] eV^{-1}
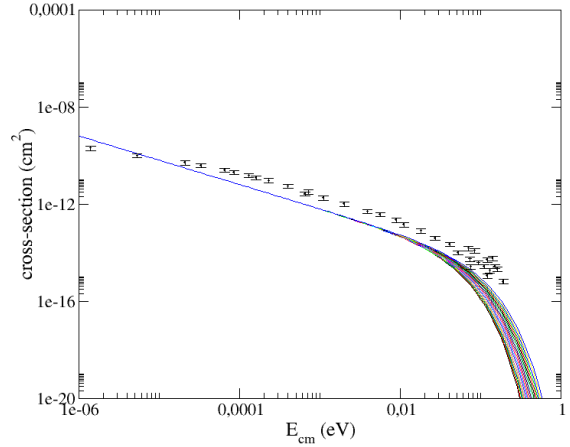
Figure 11: Influences of the different factors, in black the data points.

From Fig. 11, we can conclude that :

> A is where the curve's gonna be with respect to the y-axis, it makes a translation along this axis (obvious from the formulæ)

> p is the middle-slope of the curve (idem, obvious from the formulæ)

> E_a is the trend at low energies, if $E_a > 0$ eV, it goes down, if $E_a < 0$ eV, it goes up (then E_a here is positive)

➤ D is the trend at high energies, D is negative here.

All of this is easily provable with the formulæ, one has just to take the limiting cases.

I used a BMC routine to optimize and find the fit. I obtain Fig. 12 for the fit of the cross-section and the resulting rate constant :

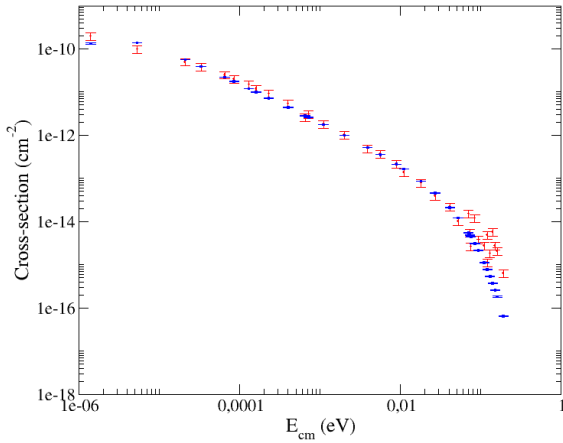➤ cross-section

    ⋈ $A = -33.15 \pm 2.10^{-2}$

    ⋈ $p = -0.897 \pm 3.10^{-3}$

    ⋈ $E_a = 2.4\,10^{-6} \pm 1.7\,10^{-7}$ eV

    ⋈ $D = -30 \pm 0.4$ eV^{-1}

    ⋈ Spearman correlation matrix :

	A	p	E_a	D
	1.00	0.47	−0.01	−0.17
	0.47	1.00	−0.20	−0.05
	−0.01	−0.20	1.00	0.18
	−0.17	−0.05	0.18	1.00

➤ Rate constant

    ⋈ $A = -10.986 \pm 2.10^{-3}$

    ⋈ $p = -0.5182 \pm 7.10^{-4}$

    ⋈ $\frac{E_a}{k_B} = 2.36 \pm 3.10^{-2}$ K

    ⋈ $D.k_B = -1.152\,10^{-3} \pm 5.10^{-6}$ K^{-1}

    ⋈ Spearman correlation matrix :

	A	p	$\frac{E_a}{k_B}$	$D.k_B$
	1.00	−0.82	0.21	0.40
	−0.82	1.00	−0.05	−0.76
	0.21	−0.05	1.00	−0.05
	0.40	−0.76	−0.05	1.00

(a) Van't Hoff BMC fit (blue) of the measured (red) cross-section
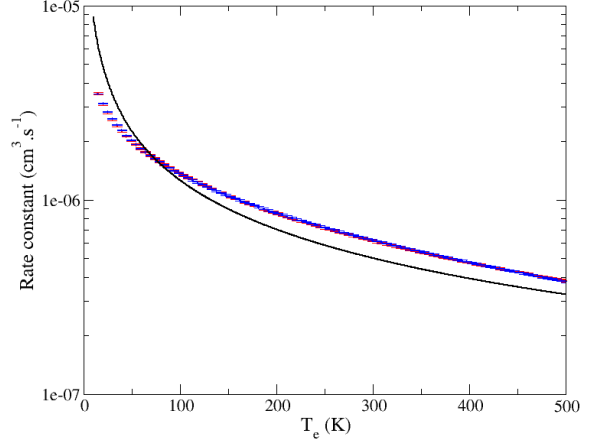
(b) α_e obtained with a Van't Hoff fit of the cross-section. Red : Calculation ; Blue : Van't Hoff fit ; black : them

Figure 12: Van't Hoff BMC fit of the cross-section and resulting rate constant

It is interesting to compare the two different calculations (Fig. 13).

It's normal than the error bars are smaller for the BMC method. It's because the all-or-nothing method accepts any parallel curve to the nominal, as it doesn't cumulate the uncertainties over the different points. It implies a lower correlation, and a wider fit. I like the fact that the better fit tends to go to higher values, I don't know yet if there's a physical interpretation or if it's just a calculation trick. I remark also that the curves are very similar, so there's maybe no need to get through the mess of fitting with the four parameters (it's not that easy...).
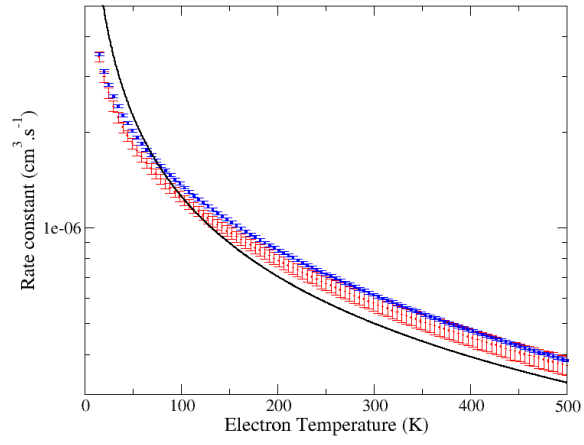
Figure 13: Red : Hercourt-Hessen, all-or-nothing fit ; blue : Van't Hoff, BMC fit ; black : them

To have an idea Of how dispersed the data might be. I take as example $C_4H_9^+$. I've taken for this species :

- $\alpha_{e0} = 8.3\,10^{-7}$ cm^3.s^{-1} with a 100 % uncertainty (no value reported), logn(8.3d-7,2)

- p varying between 0.5 and 1.5 uniformly (no value reported), unif(0.5,1.5)

This one is greatly spread (specially over the power), see Fig. 14.

(a) Rate constant (b) Rate constant at 150 K
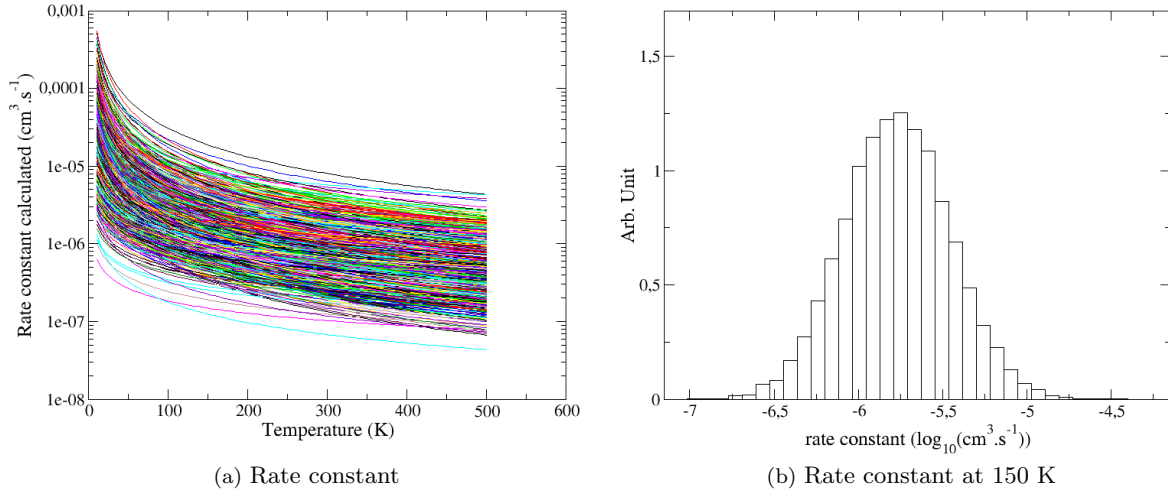
Figure 14: Rate constant obtained for $C_4H_9^+$

It's not that much... Less than the neutral species in all cases...
Let's say I put them all between 1.10^{-7} and 5.10^{-6}, with the power unif(0.5,1.5). It gives Fig. 15
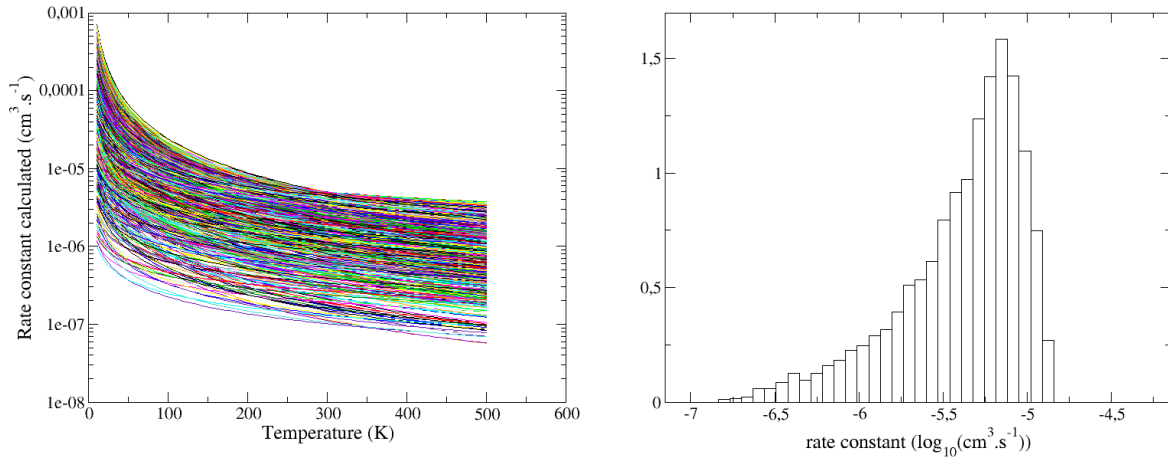
Figure 15: rate (left), rate at 150 K (right)

The change in the shape comes certainly from the change of the description of α_{e0}, change from logn to unif, it agrees well.

Conclusion   A funny paper that could explain a lot in this world...[14], in brief, they don't know what uncertainty propagation is...

4   The database

In red my personnal estimations (biggest error reported/possible/reasonnable). When big discrepancies appear, the latest version is preffered, since it's CRYRING most of the time (thinking about $C_3H_7^+$). When reasonable discrepancies appear, the most recent paper wins, with its uncertainty if overlap, a higher uncertainty so as to gain overlapping if not. It is interesting to know that, most of the time : "the errors in the branching ratios are calculated by considering the errors from the curve fitting, that is, the errors in the areas A_i (i = C + 2H, C + H, etc.), the uncertainty in the transmission, T, and the error arising from the background substraction. The errors are added in quadrature."[15] Also, "The error bars in the figure are purely statistical at the one σ level and thus represent the *relative* uncertainty, or uncertainty in the *shape* of the curve. In addition to the statistical relative uncertainties, there are also absolute systematic uncertainties which must be considered." [16]

reac	$\alpha_{e0}(\text{cm}^3.\text{s}^{-1})$	pwr	br	ref
$C^+ + e^- \rightarrow C + h\nu$	$4.67 \pm 2.33\,10^{-12}$	0.60±0.1	1	[13]
$CH^+ + e^- \rightarrow C + H$	$0.5 - 2\,10^{-7}*$	0.9±0.5	1	[6, 2, 13, 17]
$CH_2^+ + e^- \rightarrow C + H_2$	$6.4 \pm 2.0\,10^{-7}$	0.60±0.1	0.12±0.02	[15, 13, 17]
$CH_2^+ + e^- \rightarrow CH + H$	idem	idem	0.25±0.04	[15]
$CH_2^+ + e^- \rightarrow C + 2H$	idem	idem	0.63±0.06	[15]
$CH_3^+ + e^- \rightarrow CH_2 + H$	$4.72 \pm 1.2\,10^{-7}$	0.53±0.1	0.40±0.1	[18, 19, 17]
$CH_3^+ + e^- \rightarrow CH + H_2$	idem	idem	0.14±0.1	[18, 19]
$CH_3^+ + e^- \rightarrow CH + 2H$	idem	idem	0.16±0.15	[18, 19]
$CH_3^+ + e^- \rightarrow C + H_2 + H$	idem	idem	0.30±0.08	[18, 19]
$CH_4^+ + e^- \rightarrow C + 2H_2$ $CH_4^+ + e^- \rightarrow C + H_2 + 2H$ $CH_4^+ + e^- \rightarrow C + 4H$ $CH_4^+ + e^- \rightarrow CH + H_2 + H$ $CH_4^+ + e^- \rightarrow CH + 3H$ $CH_4^+ + e^- \rightarrow CH_2 + H_2$ $CH_4^+ + e^- \rightarrow CH_2 + 2H$ $CH_4^+ + e^- \rightarrow CH_3 + H$	$12.8 \pm 5\,10^{-7}$	0.5-1.5	0-1	[20]
$CH_5^+ + e^- \rightarrow CH_4 + H$	$2.8 - 11\,10^{-7}$	0.46-1.5	0.019-0.049	[21, 22, 23, 24, 25, 6, 17]
$CH_5^+ + e^- \rightarrow CH_3 + H_2$	idem	idem	0.026-0.048	[24, 6]
$CH_5^+ + e^- \rightarrow CH_3 + H + H$	idem	idem	0.65-0.70	[24, 6]
$CH_5^+ + e^- \rightarrow CH_2 + H_2 + H$	idem	idem	0.17-0.25	[24, 6]
$CH_5^+ + e^- \rightarrow CH + H_2 + H_2$	idem	idem	0.033-0.05	[24, 6]
$C_2H^+ + e^- \rightarrow C_2 + H$	$2.7 \pm 0.06\,10^{-7}$	0.76±0.02	0.43±0.03	[26, 27, 13]
$C_2H^+ + e^- \rightarrow CH + C$	idem	idem	0.39±0.04	[26, 27]
$C_2H^+ + e^- \rightarrow C + C + H$	idem	idem	0.18±0.04	[26, 27]
$C_2H_2^+ + e^- \rightarrow C_2H + H$	$2.7 \pm 0.67\,10^{-7}$	0.5±0.1	0.50±0.06	[6, 28, 13]
$C_2H_2^+ + e^- \rightarrow CH + CH$	idem	idem	0.13±0.01	[6, 28]
$C_2H_2^+ + e^- \rightarrow C_2 + 2H$	idem	idem	0.30±0.05	[6, 28]
$C_2H_2^+ + e^- \rightarrow CH_2 + CH$	idem	idem	0.05±0.01	[6, 28]
$C_2H_2^+ + e^- \rightarrow C_2 + H_2$	idem	idem	0.02±0.03	[6, 28]
$C_2H_3^+ + e^- \rightarrow C_2H_2 + H$	$4.76 \pm 1.2\,10^{-7}$	0.84±0.1	0.29±0.04	[12, 13]
$C_2H_3^+ + e^- \rightarrow C_2H + H_2$	idem	idem	0.06±0.03	[12, 13]Val. Kal. modified
$C_2H_3^+ + e^- \rightarrow C_2H + 2H$	idem	idem	0.584±0.06	for sum=1(0.59)[12]
$C_2H_3^+ + e^- \rightarrow C_2 + H + H_2$	idem	idem	0.03±0.01	[12]
$C_2H_3^+ + e^- \rightarrow CH_3 + C$	idem	idem	0.006±0.002	[12]
$C_2H_3^+ + e^- \rightarrow CH_2 + CH$	idem	idem	0.03±0.01	[12]
$C_2H_4^+ + e^- \rightarrow C_2H_3 + H$	$5.6 \pm 1.2\,10^{-7}$	0.76±0.1	0.11±0.07	[26, 27, 13]
$C_2H_4^+ + e^- \rightarrow C_2H_2 + H_2$	idem	idem	0.06±0.03	[26, 27]
$C_2H_4^+ + e^- \rightarrow C_2H_2 + H + H$	idem	idem	0.66±0.06	[26, 27]
$C_2H_4^+ + e^- \rightarrow C_2H + H_2 + H$	idem	idem	0.10±0.04	[26, 27]
$C_2H_4^+ + e^- \rightarrow CH_4 + C$	idem	idem	0.01±0.01	[26, 27]
$C_2H_4^+ + e^- \rightarrow CH_3 + CH$	idem	idem	0.02±0.02	[26, 27]
$C_2H_4^+ + e^- \rightarrow CH_2 + CH_2$	idem	idem	0.04±0.02	[26, 27]

reac	α_{e0} (cm³.s⁻¹)	pwr	br	ref
$C_2H_5^+ + e^- \rightarrow CH_3 + CH_2$	$6.7 \pm 6.7\,10^{-7}$	0.79 ± 0.1	0.17 ± 0.04	[22, 13]
$C_2H_5^+ + e^- \rightarrow C_2H_2 + H_2 + H$	idem	idem	0.31 ± 0.08	for sum=1(0.31)[13]
$C_2H_5^+ + e^- \rightarrow C_2H_3 + 2H$	idem	idem	0.27 ± 0.07	[13]
$C_2H_5^+ + e^- \rightarrow C_2H_2 + 3H$	idem	idem	0.13 ± 0.03	[13]
$C_2H_5^+ + e^- \rightarrow C_2H_4 + H$	idem	idem	0.12 ± 0.03	[13]
$C_3H_2^+ + e^- \rightarrow C_2H_2 + C$	$4.8 \pm 4.8\,10^{-7}$	0.5 ± 0.1	0.06 ± 0.06	[13]
$C_3H_2^+ + e^- \rightarrow C_3 + 2H$	idem	idem	0.12 ± 0.12	[13]
$C_3H_2^+ + e^- \rightarrow C_2 + CH_2$	idem	idem	0.06 ± 0.06	[13]
$C_3H_2^+ + e^- \rightarrow C_3H + H$	idem	idem	0.64 ± 0.40	for sum=1(0.60)[13]
$C_3H_2^+ + e^- \rightarrow C_3 + H_2$	idem	idem	0.12 ± 0.12	[13]
$c - C_3H_3^+ \rightarrow c - C_3H_2 + H$	$8.00 \pm 0.1\,10^{-7}$	1 ± 0.5	1	[29, 30]
$l - C_3H_3^+ \rightarrow l - C_3H_2 + H$	$1.15 \pm 0.02\,10^{-7}$	1 ± 0.5	1	[29, 30]
$C_3H_4^+ + e^- \rightarrow l - C_3H_3 + H$ $C_3H_4^+ + e^- \rightarrow c - C_3H_3 + H$	$2.95 \pm 0.1\,10^{-6}$	0.67 ± 0.02	0.87 ± 0.04	[31]
$C_3H_4^+ + e^- \rightarrow C_3H_2 + H_2$	idem	idem	≤ 0.02	[31]
$C_3H_4^+ + e^- \rightarrow C_2H_3 + CH$	idem	idem	0.01 ± 0.01	[31]
$C_3H_4^+ + e^- \rightarrow C_2H_2 + CH_2$	idem	idem	0.06 ± 0.02	[31]
$C_3H_4^+ + e^- \rightarrow C_2H + CH_3$	idem	idem	0.01 ± 0.01	[31]
$C_3H_4^+ + e^- \rightarrow C_3H_2 + 2H$	idem	idem	≤ 0.05	[31]
$C_3H_5^+ + e^- \rightarrow l - C_3H_3 + H_2$ $C_3H_5^+ + e^- \rightarrow c - C_3H_3 + H_2$	$3.0 \pm 3.0\,10^{-7}$	0.5 ± 0.1	0-1	[13]
$C_3H_5^+ + e^- \rightarrow CH_3CCH + H$	idem	idem	0-1	[13]
$C_3H_7^+ + e^- \rightarrow C_3H_6 + H$	$1.9 \pm 0.35\,10^{-6}$	0.68 ± 0.01	0.42 ± 0.10	[32, 26]
$C_3H_7^+ + e^- \rightarrow C_3H_5 + H_2$ $C_3H_7^+ + e^- \rightarrow C_3H_5 + H + H$	idem	idem	0.12 ± 0.08	[32, 26]
$C_3H_7^+ + e^- \rightarrow C_3H_4 + H_2 + H$	idem	idem	0.09 ± 0.05	[32, 26]
$C_3H_7^+ + e^- \rightarrow C_2H_4 + CH_3$ $C_3H_7^+ + e^- \rightarrow C_2H_4 + CH_2 + H$	idem	idem	0.04 ± 0.02	[32, 26]
$C_3H_7^+ + e^- \rightarrow C_2H_3 + CH_4$ $C_3H_7^+ + e^- \rightarrow C_2H_3 + CH_3 + H$	idem	idem	0.19 ± 0.05	[32, 26]
$C_3H_7^+ + e^- \rightarrow C_2H_2 + CH_4 + H$ $C_3H_7^+ + e^- \rightarrow C_2H_2 + CH_3 + H_2$	idem	idem	0.11 ± 0.02	[32, 26]
$C_3H_7^+ + e^- \rightarrow C_3H_3 + H_2 + H_2$ $C_3H_7^+ + e^- \rightarrow C_2H_6 + CH$ $C_3H_7^+ + e^- \rightarrow C_2H_5 + CH_2$ $C_3H_7^+ + e^- \rightarrow C_2H_4 + CH + H_2$ $C_3H_7^+ + e^- \rightarrow C_2H_3 + CH_2 + H_2$ $C_3H_7^+ + e^- \rightarrow C_2H + CH_4 + H_2$	idem	idem	≤ 0.05	[32, 26]
$C_4H_4^+ + e^- \rightarrow C_4H_3 + H$	$3.3 \pm 0.82\,10^{-7}$	0.5 ± 0.1	1	[13]
$C_4H_5^+ + e^- \rightarrow C_4$: 12 possibilities	$8.2 \pm 2.5\,10^{-7}$	0.5-1.5	0.526 ± 0.002	[7, 22, 33]
$C_4H_5^+ + e^- \rightarrow C_3 + C$: 33 possibilities	idem	idem	0.001 ± 0.002	[7, 22, 33]
$C_4H_5^+ + e^- \rightarrow C_2 + C_2$: 33 possibilities	idem	idem	0.473 ± 0.002	[7, 22, 33]
$C_4H_7^+ + e^- \rightarrow H_2CCCC + 2H_2 + H$	$3.0 \pm 3.0\,10^{-7}$	0.5 ± 0.1	1	[13]

reac	$\alpha_{e0}(\mathrm{cm}^3.\mathrm{s}^{-1})$	pwr	br	ref
$\mathrm{NH}^+ + e^- \rightarrow N + H$	$0.43-10\,10^{-7}$	0.5 ± 0.1	1	[34]
$\mathrm{NH}_2^+ + e^- \rightarrow N + H_2$	$1-10\,10^{-7}$	0.5-1.5	0.00-0.10	[6, 35, 36, 37]
$\mathrm{NH}_2^+ + e^- \rightarrow NH + H$	idem	idem	0.30-0.49	[6, 35, 36, 37]
$\mathrm{NH}_2^+ + e^- \rightarrow N + 2H$	idem	idem	0.41-0.66	[6, 35, 36, 37]
$\mathrm{N}_2\mathrm{H}^+ + e^- \rightarrow N_2 + H$	$1.0-10.0\,10^{-7}$	0.5-1.0	1	Geppert2004a corrected [38, 23, 34]
$\mathrm{CN}^+ + e^- \rightarrow N + C$	$1.8\pm1.8\,10^{-7}$	0.5 ± 0.1	1	[13]
$\mathrm{HCNH}^+ + e^- \rightarrow HCN + H$	$2.8\pm30\%\,10^{-7}$	0.65 ± 0.1	0.26-0.41**	[39, 40]
$\mathrm{HCNH}^+ + e^- \rightarrow HNC + H$	idem	idem	0.29-0.39**	[39, 40]
$\mathrm{HCNH}^+ + e^- \rightarrow CN + H_2$	idem	idem	0±0.017	[39]
$\mathrm{HCNH}^+ + e^- \rightarrow CN + 2H$	idem	idem	0.325±0.032	[39]
$\mathrm{CNC}^+ \rightarrow CN + C$	$3.0\pm3.0\,10^{-7}$	0.5 ± 0.1	1	[13]
$\mathrm{C}_2\mathrm{N}_2^+ + e^- \rightarrow CN + CN$	$3.0\pm3.0\,10^{-7}$	0.5 ± 0.1	0-1	[13]
$\mathrm{C}_2\mathrm{N}_2^+ + e^- \rightarrow C_2N + N$	idem	idem	0-1	[13]
$\mathrm{C}_3\mathrm{N}^+ + e^- \rightarrow CN + C_2$	$3.0\pm3.0\,10^{-7}$	0.5 ± 0.1	1	[13]
$\mathrm{C}_4\mathrm{N}^+ + e^- \rightarrow C_3N + C$	$3.0\pm3.0\,10^{-7}$	0.5 ± 0.1	0-1	[13]
$\mathrm{C}_4\mathrm{N}^+ + e^- \rightarrow C_2N + C_2$	idem	idem	0-1	[13]
$\mathrm{NH}_3^+ + e^- \rightarrow NH + 2H$	$3.1\pm0.8\,10^{-7}$	0.5 ± 0.1	0-1	[13]
$\mathrm{NH}_3^+ + e^- \rightarrow NH_2 + H$	idem	idem	0-1	[13]
$\mathrm{NH}_4^+ + e^- \rightarrow NH_3 + H$	$9.0-15.0\,10^{-7}$	0.47-0.9	0.69±0.03	[9, 41, 34, 35, 13]
$\mathrm{NH}_4^+ + e^- \rightarrow NH_2 + H_2$	idem	idem	0.10±0.02	[35]
$\mathrm{NH}_4^+ + e^- \rightarrow NH_2 + 2H$	idem	idem	0.21±0.03	[35]
$\mathrm{NH}_4^+ + e^- \rightarrow NH + H + H_2$	idem	idem	0.00±0.01	[35]
$\mathrm{NH}_4^+ + e^- \rightarrow N + 2H_2$	idem	idem	0.00±0.01	[35]
$\mathrm{H}_2\mathrm{O}^+ + e^- \rightarrow OH + H$	$0.5-6.0\,10^{-7}$	0.8±0.05	0.1-0.4	[34, 42, 43]
$\mathrm{H}_2\mathrm{O}^+ + e^- \rightarrow O + H_2$	idem	idem	0-0.2	[42, 43]
$\mathrm{H}_2\mathrm{O}^+ + e^- \rightarrow O + 2H$	idem	idem	0.4-0.9	[42, 43]
$\mathrm{H}_3\mathrm{O}^+ + e^- \rightarrow OH + 2H$	$4.3\pm0.6\,10^{-7}$	0.5-1.5	0.597±0.4	for sum=1 (0.60)[34, 44, 45, 18, 46]
$\mathrm{H}_3\mathrm{O}^+ + e^- \rightarrow H_2O + H$	idem	idem	0.25±0.3	[34, 44, 45, 18, 46]
$\mathrm{H}_3\mathrm{O}^+ + e^- \rightarrow OH + H_2$	idem	idem	0.14±0.1	[34, 44, 45, 18, 46]
$\mathrm{H}_3\mathrm{O}^+ + e^- \rightarrow O + H_2 + H$	idem	idem	0.013±0.03	[34, 44, 45, 18, 46]
$\mathrm{CO}^+ + e^- \rightarrow C + O$	$2.0\pm0.8\,10^{-7}$	0.55±0.07	1	[16, 47, 34, 13]
$\mathrm{HCO}^+ + e^- \rightarrow CO + H$	$3.0\pm2\,10^{-7}$	0.64±0.02	0.92±0.03	[48, 23, 4, 21, 49, 50]
$\mathrm{HCO}^+ + e^- \rightarrow C + OH$	idem	idem	0.07±0.02	[48, 23, 4, 21, 49, 50]
$\mathrm{HCO}^+ + e^- \rightarrow O + CH$	idem	idem	0.01±0.01	[48, 23, 4, 21, 49, 50]
$\mathrm{NO}^+ + e^- \rightarrow N + O$	$4.3\pm1.1\,10^{-7}$	0.37 ± 0.1	1	[13]

$* :$ $\left.\begin{array}{ll} [2] & \rightarrow \alpha_e(120K) = 1.12\,10^{-7}\mathrm{cm}^3.\mathrm{s}^{-1} \\ [6] & \rightarrow \mathrm{pwr} = 0.9 \end{array}\right\} \Rightarrow \alpha_0 = 0.5\,10^{-7}\mathrm{cm}^3.\mathrm{s}^{-1}$

$** :$ $0.77 \leq \frac{[\mathrm{HCN}]}{[\mathrm{HNC}]} \leq 1.32$ [40] and [HCN] + [HNC] = 0.675 ± 0.016 [39] + Monte Carlo propagation [myself]

| reac	$\alpha_{e0}(\mathrm{cm^3.s^{-1}})$	pwr	br	ref
$C_4H_9^+ + e^- \rightarrow \begin{cases} C_4H_8 + H \\ C_4H_7 + H_2 \\ C_4H_7 + H + H \\ C_4H_6 + H_2 + H \\ C_4H_5 + H_2 + H_2 \end{cases}$	$8.3\,10^{-7} \pm 8.3$	0.5-1.5	0.633±0.001	for sum = 1 (0.651)[22, 7, 34]
$C_4H_9^+ + e^- \rightarrow \begin{cases} C_3H_8 + CH \\ C_3H_7 + CH_2 \\ C_3H_6 + CH_3 \\ C_3H_6 + CH_2 + H \begin{cases} {}^1CH_2 \\ {}^3CH_2 \end{cases} \\ C_3H_6 + CH + H_2 \\ C_3H_5 + CH_4 \\ C_3H_5 + CH_3 + H \\ C_3H_5 + CH_2 + H_2 \begin{cases} {}^1CH_2 \\ {}^3CH_2 \end{cases} \\ C_3H_4 + CH_4 + H \\ C_3H_4 + CH_3 + H_2 \\ C_3H_3 + CH_4 + H_2 \end{cases}$	idem	idem	0.366±0.001	for sum = 1 (0.384)[7, 34]
$C_4H_9^+ + e^- \rightarrow \begin{cases} C_2H_6 + C_2H_3 \\ C_2H_6 + C_2H_2 + H \\ C_2H_6 + C_2H + H_2 \\ C_2H_5 + C_2H_4 \\ C_2H_5 + C_2H_3 + H \\ C_2H_5 + C_2H_2 + H_2 \\ C_2H_4 + C_2H_4 + H \end{cases}$	idem	idem	0.001±0.002	[7, 34]
$C_4H_9^+ + e^- \rightarrow \begin{cases} C_2H_4 + CH + CH_4 \\ C_2H_4 + CH_2 + CH_3 \\ C_2H_3 + CH_3 + CH_3 \\ C_2H_3 + CH_2 + CH_4 \\ C_2H_2 + CH_3 + CH_4 \end{cases}$	idem	idem	0.000±0.001	[34]
$C_4H_3^+ + e^- \rightarrow \begin{cases} C_4H_2 + H \\ C_4H + H_2 \\ C_4 + H + H_2 \end{cases}$	$6.2\,10^{-7} \pm 6.2$	0.5-1.5	0.76±0.08	[51, 34]
$C_4H_3^+ + e^- \rightarrow \begin{cases} C_3H_3 + C \\ C_3H_2 + CH \\ C_3H + CH_2 \end{cases}$	idem	idem	0.06±0.06	[51, 34]
$C_4H_3^+ + e^- \rightarrow \begin{cases} C_2H_3 + C_2 \\ C_2H_2 + C_2H \\ C_3 + CH_3 \end{cases}$	idem	idem	0.18±0.06	[51, 34]

reac			$\alpha_{e0}(\mathrm{cm}^3.\mathrm{s}^{-1})$	pwr	br	ref
$C_5H_3 + e^- \rightarrow$	$C_4 \Big\{$	$\rightarrow C_4H_2 + C + H$				
		$\rightarrow C_4H_2 + CH$				
	$C_3 \Big\{$	$\rightarrow C_3 + C_2H_3$				
		$\rightarrow C_3 + C_2H_2 + H$				
		$\rightarrow C_3 + C_2H + 2H$				
		$\rightarrow C_3 + C_2 + H_2 + H$				
		$\rightarrow C_3 + C_2 + 3H$				
		$\rightarrow C_3 +^1 CH_2 + CH$				
		$\rightarrow C_3 +^3 CH_2 + CH$				
		$\rightarrow C_3 +^1 CH_2 + C + H$				
		$\rightarrow C_3 +^3 CH_2 + C + H$				
		$\rightarrow C_3 + 2CH + H$				
		$\rightarrow C_3 + CH + C + 2H$				
		$\rightarrow C_3 + 2C + H_2 + H$				
		$\rightarrow C_3 + 2C + 3H$				
		$\rightarrow C_3H +^1 CH_2 + C$				
		$\rightarrow C_3H + 2CH$				
		$\rightarrow C_3H + CH + C + H$				
		$\rightarrow C_3H + 2C + H_2$				
		$\rightarrow C_3H + 2C + 2H$				
		$\rightarrow C_3H_2 + CH + C$				
		$\rightarrow C_3H_2 + 2C + H$				
		$\rightarrow C_3H_3 + 2C$				
	$C_2 \Big\{$	$\rightarrow C_2 + CH_3 + 2C$				
		$\rightarrow C_2 +^1 CH_2 + CH + C$				
		$\rightarrow C_2 +^1 CH_2 + 2C + H$				
		$\rightarrow C_2 +^3 CH_2 + 2C + H$				
		$\rightarrow C_2 + 3CH$				
		$\rightarrow C_2 + 2CH + C + H$				
		$\rightarrow C_2 + CH + 2C + H_2$	$9 \pm 3\,10^{-7}$	05-1.5	0-1	[52]
		$\rightarrow C_2 + 3C + H_2 + H$				
		$\rightarrow C_2 + 3C + 3H$				
		$\rightarrow 2C_2 + CH_3$				
		$\rightarrow C_2 +^1 CH_2 + C_2H$				
		$\rightarrow C_2 +^3 CH_2 + C_2H$				
		$\rightarrow C_2 +^1 CH_2 + C_2 + H$				
		$\rightarrow C_2 +^3 CH_2 + C_2 + H$				
		$\rightarrow C_2 + CH + C_2H_2$				
		$\rightarrow C_2 + CH + C_2H + H$				
		$\rightarrow C_2 + CH + C_2 + H_2$				
		$\rightarrow C_2 + CH + C_2 + 2H$				
		$\rightarrow C_2 + C + C_2H_3$				
		$\rightarrow C_2 + C + C_2H_2 + H$				
		$\rightarrow C_2 + C + C_2H + H_2$				
		$\rightarrow C_2 + C + C_2H + 2H$				
		$\rightarrow 2C_2 + C + H_2 + H$				
		$\rightarrow 2C_2 + C + 3H$				
		$\rightarrow 2C_2H + CH$				
		$\rightarrow 2C_2H + C + H$				
		$\rightarrow C_2H +^1 CH_2 + 2C$				
		$\rightarrow C_2H +^3 CH_2 + 2C$				
		$\rightarrow C_2H + 2CH + C$				
		$\rightarrow C_2H + CH + 2C + H$				
		$\rightarrow C_2H + 3C + H_2$				
		$\rightarrow C_2H + 3C + 2H$				
		$\rightarrow C_2H_2 + CH + 2C$				
		$\rightarrow C_2H_2 + 3C + H$				
		$\rightarrow C_2H_3 + 3C$				
		$\vdots$				

reac			$\alpha_{e0}(\mathrm{cm}^3.\mathrm{s}^{-1})$	pwr	br	ref
$C_5H_3 + e^- \rightarrow$	C	$\vdots$ $\rightarrow CH_3 + 4C$ $\rightarrow CH_2 + CH + 3C$ $\rightarrow CH_2 + 4C + H$ $\rightarrow 3CH + 2C$ $\rightarrow 2CH + 3C + H$ $\rightarrow CH + 4C + H_2$ $\rightarrow CH + 4C + 2H$ $\rightarrow 5C + H_2 + H$ $\rightarrow 5C + 3H$	$9 \pm 3\,10^{-7}$	05-1.5	0-1	[52]

5   Beware

Changes occur, for harmony purposes, I choose not to make isomer difference in dissociative recombination id it is not done in ion-neutral bimolecular reactions. The reason's quite simple, that's because those bimolecular are still leading the race in terms of fluxes and "not dummy reaction" . A reaction can't have more than 50 different channels, too bad, I don't have the branching ratios for $C_5H_3^+$ and $C_7H_5^+$, I've done $C_5H_3^+$ with the "split it in all the possible neutrals you've got" method, I obtain 73 branching ratios... I didn't even imagine what C_7H_5 can give me... There's a solution, of course, but it would change the sampling, as the only alternative is making subgroups. I need informations, of the same nature than $C_4H_9^+$, it would provide groups by carbon number, then subgroups by hydrogen distribution. I made three subgroups, on the same basis than $C_4H_9^+$, meaning, $C_4 + C$, $C_3 + C_{n<3}$, $C_2 + C_{n \leqslant 2}$ and C.
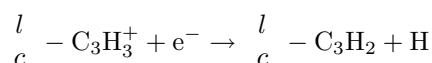
In reaction

$$C_3H_5^+ + e^- \rightarrow CH_3CCH + H$$
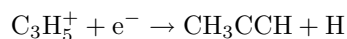
, CH_3CCH was renamed C_3H_4.

In reaction

$$C_4H_7^+ + e^- \rightarrow H_2CCCC + H_2 + H_2 + H$$

, H_2CCCC was renamed C_4H_2.

In reaction

$$\frac{l}{c} - C_3H_3^+ + e^- \rightarrow \frac{l}{c} - C_3H_2 + H$$

, the l,c difference over C_3H_2 is not taken into account yet.

6   Progs

In */home/plessis/mumuse/*, that's *fit_rate_gen.f*.

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