

1 Addition 6: Revised dissociation recombination branching ratios (2007)

After first publication of the Ethane and Propane databases [3, 4] in 2002 a number of new experimental results on dissociative recombination of hydrocarbon ions have become available, even new reaction channels have been identified. In this Section we update and revise the corresponding tables 8 and 15 in those references, respectively, for branching ratios and kinetic energy of products.

Table 1: Main dissociative recombination channels of $C_2H_y^+$, their cross section branching ratios (R_{DR}), total kinetic energy of products ($E_K^{(0)}$) in their ground states and for zero electron impact energy, and possible excited products. This table replaces Table VIII (and Table 8) of the original database Ref. [3] (and [4]), respectively.

Reaction channel	R_{DR}	$E_K^{(0)}$ (eV)	Excited products for $E \lesssim 1$ eV	
$e + C_2^+ \rightarrow C + C$	1.0	5.18	$C(^1D)$, $C(^1S)$	
$e + C_2H^+ \rightarrow C_2 + H$	0.43	5.64	$C_2(a; b; A; c; d; C)$	[5]
$\rightarrow CH + C$	0.39	2.96	$CH(A; a)$, $C(^1D; ^1S)$	
$\rightarrow C + H + C$	0.18	-0.58		$\diamond, \blacktriangledown$
$e + C_2H_2^+ \rightarrow C_2H + H$	0.50	6.53	$C_2H(A; B^1; B)$	[6]
$\rightarrow C_2 + H + H$	0.30	0.57	$C_2(a; b)$	
$\rightarrow CH + CH$	0.13	1.43	$CH(a; A)$	
$\rightarrow CH_2 + C$	0.05	2.32	$C(^1D; ^1S)$	
$\rightarrow C_2 + H_2$	0.02	5.11	$C_2(a; b; A; c; d; c)$	
$e + C_2H_3^+ \rightarrow C_2H_2 + H$	0.29	6.72		[7]
$\rightarrow C_2H + H + H$	0.59	1.85		
$\rightarrow C_2H + H_2$	0.06	6.39	$C_2H(A; B; B^1)$	
$\rightarrow CH_2 + CH$	0.03	1.18	$CH_2(a; b;)$, $CH(A; a)$	
$\rightarrow C_2 + H_2 + H$	0.024	0.43	$C_2(a; b; A)$	
$\rightarrow CH_3 + C$	0.006	2.49	$C(^1D; ^1S)$	
$e + C_2H_4^+ \rightarrow C_2H_3 + H$	0.11	5.67	$C_2H_3(A; B)$	[5]
$\rightarrow C_2H_2 + H + H$	0.66	4.15		
$\rightarrow C_2H_2 + H_2$	0.06	8.68		
$\rightarrow C_2H + H + H_2$	0.10	3.82	$C_2H(A; B'; B; C)$	
$\rightarrow CH_2 + CH_2$	0.04	3.04	$CH_2(a; b)$	
$\rightarrow CH_3 + CH$	0.02	3.44	$CH(a; A; B)$	
$\rightarrow CH_4 + C$	0.01	4.40	$C(^1D; ^1S)$	

Table 1: (continued)

Reaction channel	R_{DR}	$E_k^{(0)}$ (eV)	Excited products for $E \lesssim 1$ eV	
$e + \text{C}_2\text{H}_5^+ \rightarrow \text{C}_2\text{H}_4 + \text{H}$	(0.12)	6.53		
$\rightarrow \text{C}_2\text{H}_3 + \text{H} + \text{H}$	(0.47)	1.69	$\text{C}_2\text{H}_3(\text{A})$	
$\rightarrow \text{C}_2\text{H}_3 + \text{H}_2$	(0.06)	6.23	$\text{C}_2\text{H}_3(\text{A}; \text{B})$	
$\rightarrow \text{C}_2\text{H}_2 + \text{H}_2 + \text{H}$	(0.12)	4.70		
$\rightarrow \text{C}_2\text{H}_2 + 3\text{H}$	(0.06)	0.17		\diamond
$\rightarrow \text{CH}_4 + \text{CH}$	0.02	3.97	$\text{CH}(\text{A}; \text{a}; \text{B})$	
$\rightarrow \text{CH}_3 + \text{CH}_2$	0.15	3.92	$\text{CH}_2(\text{a}; \text{b}; \text{c})$	
$e + \text{C}_2\text{H}_6^+ \rightarrow \text{C}_2\text{H}_5 + \text{H}$	(0.16)	7.14	$\text{C}_2\text{H}_5(3\text{s}; 3\text{p})$	\otimes
$\rightarrow \text{C}_2\text{H}_4 + \text{H} + \text{H}$	(0.38)	5.55		
$\rightarrow \text{C}_2\text{H}_4 + \text{H}_2$	(0.06)	10.09	$\text{H}_2(\text{B})$	
$\rightarrow \text{C}_2\text{H}_3 + \text{H}_2 + \text{H}$	(0.18)	5.26	$\text{C}_2\text{H}_3(\text{A}; \text{B})$	
$\rightarrow \text{CH}_4 + \text{CH}_2$	(0.04)	7.43	$\text{CH}_2(\text{C}; 3\text{p})$	
$\rightarrow \text{CH}_3 + \text{CH}_3$	(0.09)	7.79	$\text{CH}_3(3\text{s}; 3\text{p}; 3\text{d})$	
$\rightarrow \text{CH}_3 + \text{CH}_2 + \text{H}$	(0.05)	2.17	$\text{CH}_2(\text{a}; \text{b})$	\diamond
$\rightarrow \text{CH}_2 + \text{CH}_2 + \text{H}_2$	(0.04)	1.86	$\text{CH}_2(\text{a}; \text{b})$	\diamond
$e + \text{C}_2\text{D}_5^+ \rightarrow \text{C}_2\text{D}_4 + \text{D}$	0.12	6.53		[8], \blacksquare , \diamond
$\rightarrow \text{C}_2\text{D}_3 + \text{D} + \text{D}$	0.28	1.69	$\text{C}_2\text{D}_3(\text{A})$	\diamond
$\rightarrow \text{C}_2\text{D}_2 + \text{D}_2 + \text{D}$	0.30	4.70		\diamond
$\rightarrow \text{C}_2\text{D}_2 + 3\text{D}$	0.13	0.25		\diamond
$\rightarrow \text{CD}_3 + \text{CD}_2$	0.17	3.92	$\text{CD}_2(\text{a}; \text{b}; \text{c})$	\diamond

- ◇ new channel, added to original database [3, 4] during revision 2007
- ▼ For $E < 0.58$ eV this channel is not open and the assumed branching ratios for $C_2 + H$ and $CH + C$ channels are 0.55 and 0.45, respectively.
- ⊗ The suggested branching ratios for $C_2H_6^+$ are in accordance with the experimental finding in Ref. [9] that the total branching ratio of all C_2 -containing channels is 0.78, and that for $CX+CY+\dots$ channels is 0.22. However, for the individual channels the suggested branching ratios within these two groups are fairly uncertain and are determined following the trends of R_{DR} in other CH_y^+ -cases.
- The presented branching ratios are for $C_2D_5^+$ from Ref. [8]. The branching ratios for $C_2H_5^+$ may be significantly different from the analogous channels in $C_2D_5^+$ as shown experimentally for the $C_3H_7^+$ and $C_3D_7^+$ DR in Refs. [10, 11]. (These are the channels when DR proceeds via a doubly excited state.)

Table 2: Main dissociative recombination channels of $C_3H_y^+$, their cross section branching ratios (R_{DR}), total kinetic energy of dissociation products ($E_k^{(0)}$) in their ground state and for zero electron impact energy, and possible excited products for $E \lesssim 1$ eV. This table replaces Table XV (and Table 15) of the original database Ref. [3] (and [4]), respectively.

Reaction channel	R_{DR}	$E_k^{(0)}$ (eV)	Excited products for $E \lesssim 1$ eV	★
$e + C_3^+ \rightarrow C_2 + C$	1.00	5.04	$C(^1D; ^1S; ^5S_2^0)$, $C_2(a; b; A; c; d; C; e)$	
$e + C_3H^+ \rightarrow C_3 + H$	0.66	6.32	$C_3(a; b; A; B; ^1S_u^+)$	
$\rightarrow C_2H + C$	0.31	4.70	$C(^1D; ^1S; ^5S_2^0)$, $C_2H(A, B^1, B)$	
$\rightarrow C_2 + CH$	0.03	2.31	$C_2(a; b; A; c; d)$, $CH(a, A)$	
$e + C_3H_2^+ \rightarrow C_3H + H$	(0.78)	9.15	$H(n=2)$	
$\rightarrow C_3 + H + H$	(0.07)	2.78	$C_3(a; b)$	
$\rightarrow C_3 + H_2$	(0.02)	7.31	$C_3(a; b; A; B; ^1S_u^+)$	
$\rightarrow C_2H_2 + C$	(0.05)	6.05	$C(^1D; ^1S; ^5S_2^0)$	
$\rightarrow C_2H + CH$	(0.06)	4.73	$CH(a; A; B; C)$, $C_2H(A; B^1; B)$	
$\rightarrow C_2 + CH_2$	(0.02)	3.20	$C_2(a; b; A; c; d)$, $CH_2(a; b; c)$	
$e + C_3H_3^+ \rightarrow C_3H_2 + H$	(0.82)	3.38	$C_3H_2(A; B)$	
$\rightarrow C_3H + H + H$	(0.06)	2.10		
$\rightarrow C_3H + H_2$	(0.03)	6.64		
$\rightarrow C_3 + H_2 + H$	0.00	—		□
$\rightarrow C_2H_2 + CH$	(0.04)	2.55	$CH(a; A)$	
$\rightarrow C_2 + CH_3$	(0.01)	1.00	$C_2(a; b; A)$	
$\rightarrow C_2H + CH_2$	(0.04)	2.11	$CH_2(a; b)$	
$e + C_3H_4^+ \rightarrow C_3H_3 + H$	0.87	7.28		[12]
$\rightarrow C_3H_2 + H + H$	0.04	2.32	$C_3H_2(A; B)$	
$\rightarrow C_3H_2 + H_2$	0.01	6.86	$C_3H_2(A; B; C)$	
$\rightarrow C_3H + H_2 + H$	0.00	—		□
$\rightarrow C_2 + CH_4$	0.00	—	$C_2(a; b; A; c; d; C)$	□
$\rightarrow C + C_2H_4$	0.00	—	$C(^1D; ^1S)$	□
$\rightarrow C_2H_3 + CH$	0.01	3.02	$CH(a; A; B)$	◇
$\rightarrow C_2H_2 + CH_2$	0.06	5.93	$CH_2(a; b; c)$	◇
$\rightarrow C_2H + CH_3$	0.01	5.91	$C_2H(A; B^1; C)$, $CH_3(A'_1)$	◇

Table 2: (continued)

Reaction channel	R_{DR}	$E_k^{(0)}$ (eV)	Excited products for $E \lesssim 1$ eV	★
$e + C_3H_5^+ \rightarrow C_3H_4 + H$	(0.72)	5.70		
$\rightarrow C_3H_3 + H + H$	(0.06)	2.63		
$\rightarrow C_3H_3 + H_2$	(0.03)	7.16		◆
$\rightarrow C_3H_2 + H_2 + H$	(0.06)	2.21	$C_3H_2(A; B)$	
$\rightarrow C_2H + CH_4$	(0.02)	5.73	$C_2H(A; B^1; B)$	
$\rightarrow C_2H + CH_3 + H$	(0.02)	1.25		◇
$\rightarrow C_2H_4 + CH$	(0.03)	3.20	$CH(a; A; B)$	
$\rightarrow C_2H_3 + CH_2$	(0.02)	2.80	$C_2H_3(A), CH_2(a; b; c)$	
$\rightarrow C_2H_2 + CH_3$	(0.03)	6.12	$CH_3(3s)$	
$\rightarrow C_2H_2 + CH_2 + H$	(0.01)	1.27	$CH_2(a; b)$	◇
$e + C_3H_6^+ \rightarrow C_3H_5 + H$	(0.53)	5.90	$C_3H_5(A; B; C; 3d)$	
$\rightarrow C_3H_4 + H + H$	(0.06)	3.47		
$\rightarrow C_3H_4 + H_2$	(0.04)	8.01		◆
$\rightarrow C_3H_3 + H_2 + H$	(0.06)	4.94		
$\rightarrow C_2H_5 + CH$	(0.04)	2.56	$CH(a; A)$	
$\rightarrow C_2H_4 + CH_2$	(0.06)	5.40	$CH_2(a; b; c);$	
$\rightarrow C_2H_3 + CH_3$	(0.09)	5.42	$C_2H_3(A; B), CH_3(3s)$	
$\rightarrow C_2H_2 + CH_4$	(0.04)	8.93		◇
$\rightarrow C_2H_2 + CH_3 + H$	(0.08)	3.89		◇
$e + C_3H_7^+ \rightarrow C_3H_6 + H$	0.42	5.97		
$\rightarrow C_3H_5 + H + H$	0.08	2.15	$C_3H_5(A)$	△
$\rightarrow C_3H_5 + H_2$	0.04	6.69	$C_3H_5(A; B; C; 3d; 4s)$	△
$\rightarrow C_3H_4 + H_2 + H$	0.09	4.27		
$\rightarrow C_2H_6 + CH$	(0.01)	3.19	$CH(a; A; B)$	▲
$\rightarrow C_2H_5 + CH_2$	(0.01)	3.24	$CH_2(a; b; c)$	▲
$\rightarrow C_2H_4 + CH_3$	0.04	6.51	$CH_3(3s; 3p)$	▽
$\rightarrow C_2H_3 + CH_4$	0.04	5.95	$C_2H_3(A; B)$	△
$\rightarrow C_2H_3 + CH_3 + H$	0.15	1.67	$C_2H_3(A)$	△, ◇
$\rightarrow C_2H_2 + CH_4 + H$	(0.01)	4.62		◇, ▲
$\rightarrow C_2H_2 + CH_3 + H_2$	0.11	4.68		◇, ▲

Table 2: (continued)

Reaction channel	R_{DR}	$E_k^{(0)}$ (eV)	Excited products for $E \lesssim 1$ eV	★
$e + C_3H_8^+ \rightarrow C_3H_7 + H$	(0.46)	6.67	$C_3H_7(3s; 3p; 3d)$	
$\rightarrow C_3H_6 + H + H$	(0.09)	5.10		
$\rightarrow C_3H_6 + H_2$	(0.05)	9.63	$H_2(B)$	
$\rightarrow C_3H_5 + H_2 + H$	(0.08)	5.82	$C_3H_5(A; B; C; 3d)$	
$\rightarrow C_2H_6 + CH_2$	(0.07)	6.74	$CH_2(a; b; c)$	
$\rightarrow C_2H_5 + CH_3$	(0.06)	7.22	$CH_3(3s; 3p), C_2H_5(3s; 3p)$	
$\rightarrow C_2H_4 + CH_4$	(0.01)	10.11		◇
$\rightarrow C_2H_4 + CH_3 + H$	(0.08)	5.63	$CH_3(3s)$	◇
$\rightarrow C_2H_3 + CH_4 + H$	(0.03)	5.28	$C_2H_3(A; B)$	◇
$\rightarrow C_2H_3 + CH_3 + H_2$	(0.06)	5.33	$CH_3(3s); C_2H_3(A; B)$	◇
$\rightarrow C_2H_2 + CH_4 + H_2$	(0.01)	8.28		◇

★ The values of R_{DR} given in parentheses are suggested by using the trend of R_{DR} for the analogous DR channels in systems where R_{DR} have been measured at $E \simeq 0$ eV ($C_3H_4^+$, $C_3H_7^+$), as well as some other physical considerations. The assigned values for R_{DR} , however, satisfy the experimental findings for the weights of $[C_3^+]$ and $[C_2] + [C]$ in the total DR of Ref. [9].

□ channel removed from database [3, 4], during revision 2007

◇ new channel, added to original database [3, 4] during revision 2007

◆ This channel is only open for $E \gtrsim 1$ eV.

△ The measured combined branching ratio for these reactions [8] was partitioned among them in accordance with the weights of branching ratios of analogous reactions in the $C_3D_7^+$ case [10].

▲ The combined branching ratio for these reactions was found to be < 0.05 in Ref. [8]. In the $C_3D_7^+$ case the DR channels $C_2D_2 + CD$ and $C_2D_5 + CD_2$ have not been detected [10].

▽ It is possible that $C_2H_4 + CH_2 + H$ channel contributes to the R_{DR} value by 0.01 or less. This channel, however, has not been detected in the $C_3D_7^+$ case [10].

References

- [1] R. K. Janev and D. Reiter, *Phys. Plasmas* **9**, 4071 (2002)
- [2] 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).
- [3] R. K. Janev and D. Reiter, *Phys. Plasmas* **11**, 780 (2004);
- [4] 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).
- [5] A. Ehlerding, F. Hellberg, R. Thomas et al., *Phys. Chem. Lett.* **6**, 949 (2004)
- [6] A. M. Derkatch, A. Al-Khalili, L. Viktor et al., *J. Phys. B* **32**, 3391 (1999)
- [7] S. Kalthori, A.A. Viggiano, S. T. Arnold et al., *Astron. Astrophys.* **391**, 1159 (2002)
- [8] W. Geppert, A. Ehlerding, F. Hellberg et al., *Phys. Rev. Lett.* **93**, 153201 (2004)
- [9] G. Angelova, O. Novotny, J.B.A. Mitchell et al., *Int. J. Mass Spectrom.* **235**, 7 (2004)
- [10] A. Ehlerding, S. T. Arnold, A. A. Viggiano et al., *J. Phys. Chem. A* **107**, 2179 (2003)
- [11] M. Larsson, A. Ehlerding, W. D. Geppert et al., *J. Chem. Phys.* **122**, 156101 (2005)
- [12] W.D. Geppert, R. Thomas, A. Ehlerding et al., *Int. J. Mass Spectrom.* **237**, 25 (2004)