PCCP

CORRECTION

View Article Online
View Journal | View Issue

Cite this: *Phys. Chem. Chem. Phys.*, 2018, **20**, 28941

DOI: 10.1039/c8cp91898h

rsc.li/pccp

Correction: Reactive polycyclic aromatic hydrocarbon dimerization drives soot nucleation

M. R. Kholghy, G. A. Kelesidis and S. E. Pratsinis*

Correction for 'Reactive polycyclic aromatic hydrocarbon dimerization drives soot nucleation' by M. R. Kholghy *et al.*, *Phys. Chem. Chem. Phys.*, 2018, **20**, 10926–10938.

The authors would like to make the following corrections to the published article.

(1) In the Nomenclature, the following should be added:

A_v	Avogadro number [mole^{-1}]

(2) On page 10928, eqn (1) and (2) should be changed as follows. In the correct format, the changes are shown in bold.

Wrong format	Correct format
$k_f = 2.2\mathcal{P}10^6 d_{ij}^2\sqrt{8\pi k_B/\mu_{ij}}T^{0.5}$	$k_f = 2.2\mathcal{P}\boldsymbol{A_v}10^6 d_{ij}^2\sqrt{8\pi k_B/\mu_{ij}}T^{0.5}$
$k_r = 2.2\mathcal{P}10^{6-b} d_{ij}^2\sqrt{8\pi k_B/\mu_{ij}}T^{0.5}e^{(-a\varepsilon\ln b/R_u T)}$	$k_r = 2.2\mathcal{P}\boldsymbol{A_v}10^{6-b} d_{ij}^2\sqrt{8\pi k_B/\mu_{ij}}T^{0.5}e^{(-a\varepsilon\ln \boldsymbol{10}/R_u T)}$

This change will affect some formulas listed in Table 1 of page 10928. The changes are shown in bold.

Table 1 Rate coefficients in Arrhenius form: $k = AT^n\exp(-E/RT)$. Units are cm^3, K, mol, s, and kcal

Type	#	Reaction	A		n	E	Ref.
Reversible dimerization	1	$PAH_i + PAH_j \Leftrightarrow Dimer^*_{ij}$	f	$2.2\mathcal{P}\boldsymbol{A_v}10^6 d_{ij}^2\sqrt{8\pi k_B/\mu_{ij}}$	0.5	0.0	This work
			r	$2.2\mathcal{P}\boldsymbol{A_v}10^{6-b} d_{ij}^2\sqrt{8\pi k_B/\mu_{ij}}$	0.5	$a\varepsilon\ln\boldsymbol{10}$	This work
	2	$PAH_i + PAH_{j\_}1 \Leftrightarrow Dimer^*_{ij\_}1$	f	$2.2\mathcal{P}\boldsymbol{A_v}10^6 d_{ij}^2\sqrt{8\pi k_B/\mu_{ij}}$	0.5	0.0	This work
			r	$2.2\mathcal{P}\boldsymbol{A_v}10^{6-b} d_{ij}^2\sqrt{8\pi k_B/\mu_{ij}}$	0.5	$a\varepsilon\ln\boldsymbol{10}$	This work
Dehydrogenation	3	$Dimer^*_{ij} + H \Leftrightarrow Dimer^*_{ij\_}1 + H_2$	f	10^8	1.8	16.35	52, 53
			r	8.68×10^4	2.36	6.09	53
	4	$Dimer^*_{ij} + OH \Leftrightarrow Dimer^*_{ij\_}1 + H_2O$	f	6.72×10^1	3.33	1.46	53
			r	6.44×10^{-1}	3.79	6.68	53
	5	$Dimer^*_{ij} \Leftrightarrow Dimer^*_{ij\_}1 + H$	f	1.13×10^{16}	−0.06	113.8	53
			r	4.17×10^{13}	0.15	0.0	53
Dimer bond formation	6	$PAH_{i\_}1 + PAH_{j\_}1 \Rightarrow Dimer_{ij}$	f	10^9	0.0	11.5	54
	7	$Dimer^*_{ij\_}1 \Rightarrow Dimer_{ij} + H$	f	10^{11}	0.0	21.9	53, 54
	8	$Dimer^*_{ij} \Rightarrow Dimer_{ij} + H_2$	f	10^8	0.0	36.5	54

Particle Technology Laboratory, Institute of Process Engineering, Department of Mechanical and Process Engineering, ETH Zürich, Sonneggstrasse 3, Zürich CH-8092, Switzerland. E-mail: sotiris.pratsinis@ptl.mavt.ethz.ch

(3) On page 10928, right column after eqn (3):

Wrong value of a	Correct value of a
where $a = 0.38$ and $b = 1.8$	where $a = \mathbf{0.115}$ and $b = 1.8$

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.