



Correction: Reactive polycyclic aromatic hydrocarbon dimerization drives soot nucleation

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

Cite this: *Phys. Chem. Chem. Phys.*, 2018, 20, 28941Correction for 'Reactive polycyclic aromatic hydrocarbon dimerization drives soot nucleation' by M. R. Kholghy *et al.*, *Phys. Chem. Chem. Phys.*, 2018, 20, 10926–10938.

DOI: 10.1039/c8cp91898h

rsc.li/pccp

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

$$k_f = 2.2\mathcal{P}10^6 d_{ij}^2 \sqrt{8\pi k_B / \mu_{ij}} T^{0.5}$$

$$k_r = 2.2\mathcal{P}10^{6-b} d_{ij}^2 \sqrt{8\pi k_B / \mu_{ij}} T^{0.5} e^{(-ae \ln b / R_u T)}$$

Correct format

$$k_f = 2.2\mathcal{P}A_v 10^6 d_{ij}^2 \sqrt{8\pi k_B / \mu_{ij}} T^{0.5}$$

$$k_r = 2.2\mathcal{P}A_v 10^{6-b} d_{ij}^2 \sqrt{8\pi k_B / \mu_{ij}} T^{0.5} e^{(-ae \ln 10 / R_u T)}$$

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 cm³, K, mol, s, and kcal

Type	#	Reaction	<i>A</i>	<i>n</i>	<i>E</i>	Ref.	
Reversible dimerization	1	$\text{PAH}_i + \text{PAH}_j \rightleftharpoons \text{Dimer}_{ij}^*$	<i>f</i>	$2.2\mathcal{P}A_v 10^6 d_{ij}^2 \sqrt{8\pi k_B / \mu_{ij}}$	0.5	0.0	This work
			<i>r</i>	$2.2\mathcal{P}A_v 10^{6-b} d_{ij}^2 \sqrt{8\pi k_B / \mu_{ij}}$	0.5	$ae \ln 10$	This work
	2	$\text{PAH}_i + \text{PAH}_{j-1} \rightleftharpoons \text{Dimer}_{ij-1}^*$	<i>f</i>	$2.2\mathcal{P}A_v 10^6 d_{ij}^2 \sqrt{8\pi k_B / \mu_{ij}}$	0.5	0.0	This work
			<i>r</i>	$2.2\mathcal{P}A_v 10^{6-b} d_{ij}^2 \sqrt{8\pi k_B / \mu_{ij}}$	0.5	$ae \ln 10$	This work
Dehydrogenation	3	$\text{Dimer}_{ij}^* + \text{H} \rightleftharpoons \text{Dimer}_{ij-1}^* + \text{H}_2$	<i>f</i>	10^8	1.8	16.35	52, 53
			<i>r</i>	8.68×10^4	2.36	6.09	53
	4	$\text{Dimer}_{ij}^* + \text{OH} \rightleftharpoons \text{Dimer}_{ij-1}^* + \text{H}_2\text{O}$	<i>f</i>	6.72×10^1	3.33	1.46	53
			<i>r</i>	6.44×10^{-1}	3.79	6.68	53
	5	$\text{Dimer}_{ij}^* \rightleftharpoons \text{Dimer}_{ij-1}^* + \text{H}$	<i>f</i>	1.13×10^{16}	-0.06	113.8	53
			<i>r</i>	4.17×10^{13}	0.15	0.0	53
Dimer bond formation	6	$\text{PAH}_{i-1} + \text{PAH}_{j-1} \Rightarrow \text{Dimer}_{ij}$	<i>f</i>	10^9	0.0	11.5	54
	7	$\text{Dimer}_{ij-1}^* \Rightarrow \text{Dimer}_{ij} + \text{H}$	<i>f</i>	10^{11}	0.0	21.9	53, 54
	8	$\text{Dimer}_{ij}^* \Rightarrow \text{Dimer}_{ij} + \text{H}_2$	<i>f</i>	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.

