

CORRECTION

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Correction: Molecular dynamics simulation study of distribution and dynamics of aqueous solutions of uranyl ions: the effect of varying temperature and concentration

 Manish Chopra^a and Niharendu Choudhury^{*b}

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 Correction for 'Molecular dynamics simulation study of distribution and dynamics of aqueous solutions of uranyl ions: the effect of varying temperature and concentration' by Manish Chopra *et al.*, *Phys. Chem. Chem. Phys.*, 2015, 17, 27840–27850.

The authors would like to correct the units provided for the diffusion coefficients in Tables 2, 3, 4 and 5 of the published article which should read as $10^{-5} \text{ cm}^2 \text{ s}^{-1}$, as seen in the amended Tables below.

Table 2 Diffusion coefficient values of overall water molecules at different temperatures for U1, U5 and U10 systems

 Diffusion coefficients, $D_{\text{PBC}} (10^{-5} \text{ cm}^2 \text{ s}^{-1})$ of overall water molecules

	240 K	270 K	298 K	330 K	360 K
U1	1.82	3.43	5.28	7.51	9.60
U5	1.59	2.98	4.50	6.42	8.01
U10	1.36	2.45	3.58	4.88	6.27

Table 3 Diffusion coefficient values of water molecules within first coordination shell of uranyl ions at different temperatures for U1, U5 and U10 systems

 Diffusion coefficients, $D_{\text{PBC}} (10^{-5} \text{ cm}^2 \text{ s}^{-1})$ of coordination shell water molecules

	240 K	270 K	298 K	330 K	360 K
U1	0.56	0.93	1.86	2.19	2.94
U5	0.54	0.86	1.35	2.09	2.44
U10	0.43	0.75	1.20	1.61	1.94

Table 4 Diffusion coefficient values for uranium atom of uranyl ions at different temperatures for U1, U5 and U10 systems

 Diffusion coefficients, $D_{\text{PBC}} (10^{-5} \text{ cm}^2 \text{ s}^{-1})$ for uranium atom of uranyl ion

	240 K	270 K	298 K	330 K	360 K
U1	0.46	0.76	1.37	1.89	2.43
U5	0.36	0.70	1.09	1.63	2.12
U10	0.29	0.55	0.87	1.19	1.46

^a Radiation Safety Systems Division, Bhabha Atomic Research Centre, Mumbai – 400 085, India

^b Theoretical Chemistry Section, Bhabha Atomic Research Centre, Mumbai – 400 085, India. E-mail: nihcho@barc.gov.in; Fax: +91 22-2551 5151; Tel: +91 22-2559 5089


Table 5 Diffusion coefficient values of water molecules and uranyl ions corrected for system size at different temperatures for U1, U5 and U10 systems

	240 K	270 K	298 K	330 K	360 K
Corrected diffusion coefficients, D_o ($10^{-5} \text{ cm}^2 \text{ s}^{-1}$) of overall water molecules					
U1	2.25	4.01	6.07	8.59	10.98
U5	2.02	3.56	5.29	7.50	9.39
U10	1.79	3.03	4.37	5.96	7.65
Corrected diffusion coefficients, D_o ($10^{-5} \text{ cm}^2 \text{ s}^{-1}$) of coordination shell water molecules					
U1	0.99	1.51	2.65	3.27	4.32
U5	0.97	1.44	2.26	3.17	3.82
U10	0.86	1.33	1.99	2.69	3.32
Corrected diffusion coefficients, D_o ($10^{-5} \text{ cm}^2 \text{ s}^{-1}$) of uranium atom of uranyl ions					
U1	0.89	1.34	2.16	2.97	3.81
U5	0.79	1.28	1.88	2.71	3.50
U10	0.72	1.13	1.66	2.27	2.84

In addition, on page 27848, 4th line above Table 5, the value $2.3 \times 10^{-9} \text{ cm}^2 \text{ s}^{-1}$ should actually be $2.3 \times 10^{-5} \text{ cm}^2 \text{ s}^{-1}$.
The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

