



Cite this: *Phys. Chem. Chem. Phys.*,  
2016, 18, 30877

## Correction: Simulations of the water exchange dynamics of lanthanide ions in 1-ethyl-3-methylimidazolium ethyl sulfate ([EMIm][EtSO<sub>4</sub>]) and water

Yi-Jung Tu, Matthew J. Allen and G. Andrés Cisneros\*

DOI: 10.1039/c6cp90231f

[www.rsc.org/pccp](http://www.rsc.org/pccp)

Correction for 'Simulations of the water exchange dynamics of lanthanide ions in 1-ethyl-3-methylimidazolium ethyl sulfate ([EMIm][EtSO<sub>4</sub>]) and water' by Yi-Jung Tu *et al.*, *Phys. Chem. Chem. Phys.*, 2016, DOI: 10.1039/c6cp04957e.

In the print and on-line versions of the manuscript an error was introduced in the production stage that resulted in the change of the values of the water exchange time for all three computed Lanthanide cations in the caption for Fig. 5 and in the text in page 8. The text with the correct values is below:

p. 7, Fig. 5. The caption should read: "(a) The definition of dihedral angle  $\phi(S1-S2-S3-Ln)$ : a lanthanide ion deviates from the S1-S2-S3 plane by  $\phi(S1-S2-S3-Ln)$ . (b) MD snapshots for a water-exchange event around  $Ho^{3+}$  in water/[EMIm][EtSO<sub>4</sub>]. From  $t = 0$  to 1314 ps,  $Ho^{3+}$  forms a 9-coordinate complex with [EtSO<sub>4</sub>]<sup>−</sup> anions and water molecules in the first coordination shell. The green water leaves the first coordination sphere at 1316 ps and stays in the second or the third coordination spheres until 1737 ps. The green water joins the first solvation shell again at 1739 ps, and a water exchange is complete. This reaction follows a dissociative pathway."

p. 8, left column, the second sentence of the last paragraph: should read: "For the dissociation of a water molecule, the average time it took was 1329 ps for  $Ho^{3+}$ , 2382 ps for  $Dy^{3+}$ , and 3984 ps for  $Gd^{3+}$ ."

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

