Catalysis
Science &
Technology

CORRECTION

View Article Online
View Journal | View Issue

Cite this: *Catal. Sci. Technol.*, 2014, **4**, 4099

DOI: 10.1039/c4cy90045f

www.rsc.org/catalysis

Correction: Mechanistic analysis of water oxidation catalyzed by mononuclear copper in aqueous bicarbonate solutions

Stuart G. Winikoff and Christopher J. Cramer*

Correction for 'Mechanistic analysis of water oxidation catalyzed by mononuclear copper in aqueous bicarbonate solutions' by Stuart G. Winikoff *et al., Catal. Sci. Technol.*, 2014, **4**, 2484–2489.

While all pK_a values and reduction potentials in Fig. 1 of the original paper are correct, the equilibrium percentages reported for the speciation of compounds **1**, **2**, and **3** and for compounds **4**, **6**, and **8** that derive therefrom are not. Instead, the aqueous speciation of **1**, **2**, and **3** at pH = 8.2 should be listed as 60.7%, 36.8%, and 2.5%, respectively. The aqueous speciation of **4**, **6**, and **8** is not conveniently expressed in percentages; rather, the relative equilibrium free energies for these compounds in aqueous solution are 15.2, 7.2, and 0.0 kcal mol^{-1}, respectively. Assuming small barriers to incorporation/release of water as a ligand, the replenishment of compound **4** from compound **8** will have an activation free energy about equal to that originally assigned to the rate-determining process in the catalytic cycle, namely, O–O bond formation leading to compound **13** (15.7 kcal mol^{-1}). The authors regret the errors in the originally reported percentages.

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

Department of Chemistry, Chemical Theory Center, and Supercomputing Institute, 207 Pleasant St. SE, Minneapolis, MN 55455, USA. E-mail: cramer@umn.edu