

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.

