



Cite this: *Phys. Chem. Chem. Phys.*,
2016, **18**, 31337

Correction: Benchmark thermochemistry of chloramines, bromamines, and bromochloramines: halogen oxidants stabilized by electron correlation

Daniela Trogolo and J. Samuel Arey*†

DOI: 10.1039/c6cp90261h

www.rsc.org/pccp

Correction for 'Benchmark thermochemistry of chloramines, bromamines, and bromochloramines: halogen oxidants stabilized by electron correlation' by Daniela Trogolo *et al.*, *Phys. Chem. Chem. Phys.*, 2015, **17**, 3584–3598.

Due to an overlooked arithmetic error, our previously published article contains the following erroneous statements. These errors primarily affect the thermochemical data published for NBr_2Cl .

For the last entry of the second column of Table 6, the value 95.21 should be replaced with 71.76.

For the last entry of the second column of Table 7, the value 91.00 should be replaced with 67.55.

For the last entry of the second column of Table 8, the value 93.46 should be replaced with 70.01.

In Section 3.4, in the sentence, “ $\Delta_f H_{298\text{K}}^{0,\text{TA14},\text{Best}}$ values range from 12.04 kcal mol^{−1} to 91.00 kcal mol^{−1} for chloramines, bromamines and bromochloramines (Table 7).”, the value “91.00” should be replaced with “73.82”.

In Section 3.5, in the sentence, “Halamine formation is endergonic with respect to the elemental forms at standard state, with $\Delta_f G_{298\text{K}}^{0,\text{TA14},\text{Best}}$ values ranging from 19.39 kcal mol^{−1} to 93.46 kcal mol^{−1}”, the value “93.46” should be replaced with “73.15”.

In Section 4, in the sentence, “For comparison, Morris and Isaac⁹ proposed an experimental value of 11.3 for the equilibrium constant, $K_{\text{eq, aq}}^{\text{Expt}}$ of monochloramine generation in aqueous phase (eqn (21)), derived from the ratio of the experimental forward rate constant, k_f , with the experimental reverse rate constant, k_r ”, the term “ $K_{\text{eq, aq}}^{\text{Expt}}$ ” should be replaced with “ $\log K_{\text{eq, aq}}^{\text{Expt}}$ ”.

These changes do not otherwise affect the conclusions or discussion in the article.

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

Environmental Chemistry Modeling Laboratory, École Polytechnique Fédérale de Lausanne (EPFL), Station 2, 1015 Lausanne, Switzerland

† Current address: Department of Environmental Chemistry, Eawag, Swiss Federal Institute of Aquatic Science and Technology, Überlandstrasse 133, 8600 Dübendorf, Switzerland. E-mail: samuel.arey@eawag.ch; Fax: +41 58 765 5802; Tel: +41 58 765 5482

