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CORRECTION

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Cite this: *Phys. Chem. Chem. Phys.*, 2024, **26**, 20717

Correction: Simple, accurate, adjustable-parameter-free prediction of NMR shifts for molecules in solution

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DOI: 10.1039/d4cp90128b

rsc.li/pccp

Correction for 'Simple, accurate, adjustable-parameter-free prediction of NMR shifts for molecules in solution' by Emlyn M. Hoyt *et al.*, *Phys. Chem. Chem. Phys.*, 2023, **25**, 9952–9957, https://doi.org/10.1039/D3CP00721A.

Eqn (2) and (3) were displayed incorrectly. The correct equations are shown here:

$$m = \frac{\delta_{\mathrm{expt}}(1) - \delta_{\mathrm{expt}}(2)}{\sigma_{\mathrm{calc}}(1) - \sigma_{\mathrm{calc}}(2)} \tag{2}$$

$$b = \frac{\sigma_{\mathrm{calc}}(1)\delta_{\mathrm{expt}}(2) - \sigma_{\mathrm{calc}}(2)\delta_{\mathrm{expt}}(1)}{\sigma_{\mathrm{calc}}(1) - \sigma_{\mathrm{calc}}(2)} \tag{3}$$

Additionally, the *y*-axis labels in Fig. 1 were shown incorrectly. The correct figure is shown herein.

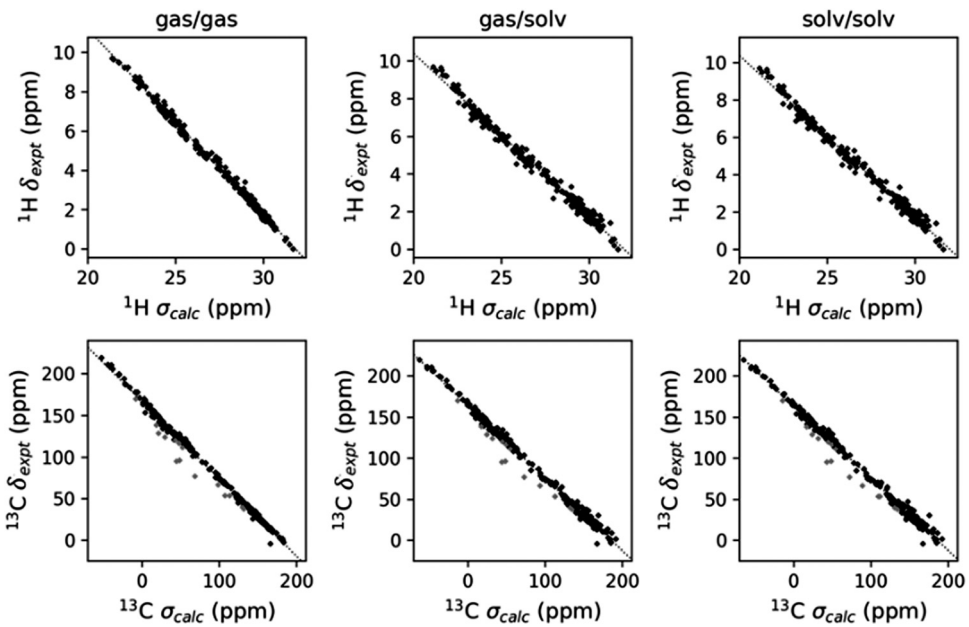

Fig. 1 Computed (B3LYP/pcS-2) shieldings *vs.* experimental shifts for ^{1}H (top) and ^{13}C (bottom) nuclei. Shieldings were computed (left) in the gas phase, (middle) applying a continuum solvation model at the gas phase optimized geometry, and (right) with a continuum solvation model applied throughout. Data points corresponding to ^{13}C nuclei adjacent to sulfur or chlorine atoms are shaded grey.

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

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