PCCP

ROYAL SOCIETY OF CHEMISTRY

CORRECTION

View Article Online
View Journal

Cite this: DOI: 10.1039/d6cp90098d

Correction: Capturing electronic substituent effect with effective atomic orbitals

Gerard Comas-Vilà and Pedro Salvador*

Correction for 'Capturing electronic substituent effect with effective atomic orbitals' by Gerard Comas-Vilà and Pedro Salvador, *Phys. Chem. Chem. Phys.*, 2025, **27**, 10482-10491, https://doi.org/10.1039/D5CP01299F.

DOI: 10.1039/d6cp90098d

rsc.li/pccp

The authors regret that two equations in the original manuscript contained errors. The correct equations are shown below.

In eqn (10), the coefficient for the I^X descriptor was incorrectly printed as 53.58. The correct coefficient is 53.38. The corrected eqn (10) is:

$$\sigma_m = 53.38I^X + 5.12R^X + 0.053 \quad (r^2 = 0.950).$$

In eqn (12), two numerical values were inadvertently exchanged. The original equation was:

$$\sigma_p = 10.17I^X + 63.36R^X + 0.018 \quad (r^2 = 0.926).$$

The corrected eqn (12) is:

$$\sigma_p = 63.36I^X + 10.17R^X + 0.018 \quad (r^2 = 0.926).$$

Additional information and clarification

To prevent potential confusion regarding the descriptors, the authors wish to clarify that, as stated in the original paper, the fits in eqn (10) and (12) were originally obtained using I^X and R^X descriptors calculated for *meta*- and *para*-benzoic acid derivatives, respectively (provided in the SI). To facilitate the direct use of values reported in Table 1 (calculated for monosubstituted benzene derivatives), the following equivalent fittings are provided:

$$\sigma_m = 52.60I^X + 5.74R^X + 0.030 \quad (r^2 = 0.937)$$

and

$$\sigma_p = 37.07I^X + 16.26R^X + 0.014 \quad (r^2 = 0.942)$$

The authors confirm that these corrections do not change the scientific conclusions of the paper. The authors apologize for any inconvenience caused.

The Royal Society of Chemistry apologises for this error and any consequent inconvenience to authors and readers.

Institut de Química Computacional i Catàlisi, Departament de Química, Universitat de Girona, c/M Aurelia Capmany 69, 17003, Girona, Catalonia, Spain.
E-mail: pedro.salvador@udg.edu