PCCP

ROYAL SOCIETY OF CHEMISTRY

CORRECTION

View Article Online
View Journal | View Issue

Cite this: *Phys. Chem. Chem. Phys.*, 2022, **24**, 4683

Correction: An integrated protocol to study hydrogen abstraction reactions by atomic hydrogen in flexible molecules: application to butanol isomers

David Ferro-Costas,*[a] M. Natália D. S. Cordeiro[b] and Antonio Fernández-Ramos*[a]

DOI: 10.1039/d2cp90022j

rsc.li/pccp

Correction for 'An integrated protocol to study hydrogen abstraction reactions by atomic hydrogen in flexible molecules: application to butanol isomers' by David Ferro-Costas *et al.*, *Phys. Chem. Chem. Phys.*, 2022, DOI: 10.1039/d1cp03928h.

The published version of this manuscript contained errors in an expression on the sixth page, in the penultimate paragraph of the Current protocol section. The correct sentence and expression is:

Therefore, the barrier height between a reactant conformer j and a TS conformer $j_{\ddagger}$ within a CRC, which at the DFT level is given by $V_0^{\mathrm{DFT}} + U_{j\ddagger}^{\mathrm{DFT}} - U_j^{\mathrm{DFT}}$, is now given by $V_0^{\mathrm{F12}} + U_{j\ddagger}^{\mathrm{DFT}} - U_j^{\mathrm{DFT}}$.

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

[a] *Center for Research in Biological Chemistry and Molecular Materials (CIQUS), University of Santiago de Compostela, 15782, Santiago de Compostela, Spain. E-mail: david.ferro@usc.es, qf.ramos@usc.es*
[b] *LAQV@REQUIMTE, Department of Chemistry & Biochemistry, Faculty of Sciences, University of Porto, Rua do Campo Alegre, 4169-007, Porto, Portugal*