Correction: Hydrogen-activation mechanism of [Fe] hydrogenase revealed by multi-scale modeling

Arndt Robert Finkelmann,*a Hans Martin Senn*b and Markus Reiher*a

Correction for ‘Hydrogen-activation mechanism of [Fe] hydrogenase revealed by multi-scale modeling’ by Arndt Robert Finkelmann et al., Chem. Sci., 2014, 5, 4474–4482, DOI: 10.1039/C4SC01605J.

The authors regret that there were minor typographical errors in two figures. In Fig. 9 and 11, the internuclear distances were swapped. The Fe-bound hydrogen atoms are affected, where Hp is the hydrogen atom proximal to the oxypyridine ligand and Hd is the hydrogen atom distal to the oxypyridine ligand. In Fig. 9, left panel, the distance between Hp and the oxypyridine O atom was given as 1.82 Å and the distance between Hp and the Fe atom was given as 1.7 Å. However, it should read 1.82 Å between Hp and Fe and 1.70 Å between Hp and the oxypyridine O atom. In Fig. 11, top left panel, the distance between Hp and Fe was shown to be 1.70 Å and the distance between Hd and Fe was given as 1.73 Å. However, it should read 1.73 Å between Hp and Fe and 1.70 Å between Hd and Fe. The correct versions of these figures are given below. The results and conclusions are not affected by these typographical errors.

Fig. 9  QM/MM-optimized reactant (left) and product (right) structures of the H₂ cleavage reaction for the scenario with oxypyridine ligand. Distances are given in Å.
Fig. 11  Top row: structures of the H₂ adduct for the second scenario with neutral pyridinol; the pyridinol OH can be oriented away from Fe (top left) or towards Fe (top right). Bottom row: products of H₂ cleavage, with the proton transferred to the thiolate; with the hydroxyl oriented away from Fe (bottom left) and towards Fe (bottom right). Distances are given in Å; relative energies with respect to the favoured adduct are indicated in red in kcal mol⁻¹.

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