Proton transfer reactions and dynamics in protonated water clusters

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The figure shown below replaces Figure 1 on page 7 of the published article.

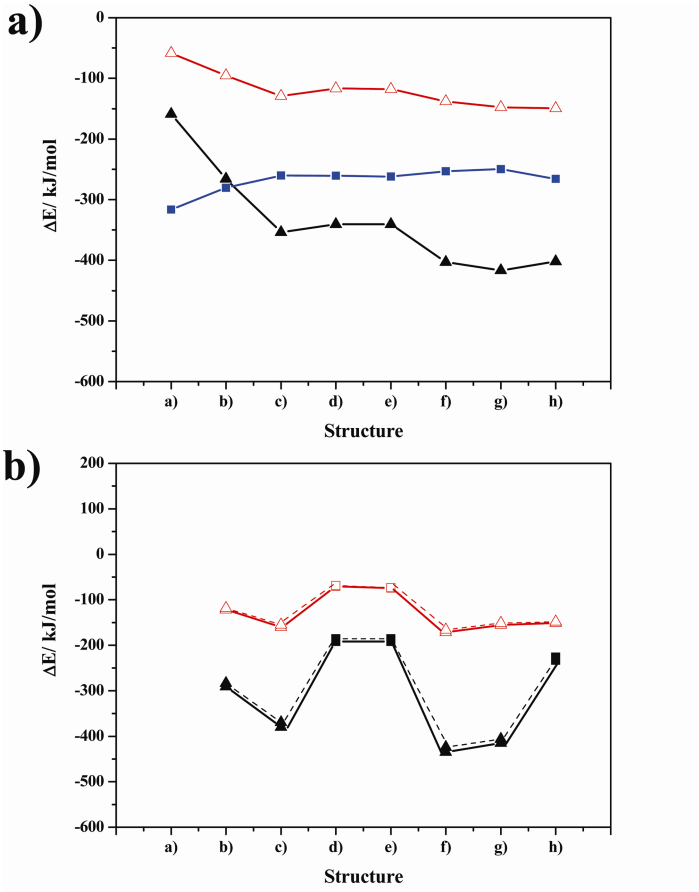

Fig. 1 (a) Trends of the interaction (ΔE) and solvation energies (ΔE^{sol}) with respect to the number of water molecules, obtained from B3LYP/TZVP calculations: -▲- = ΔE in the gas phase; -△- = ΔE in continuum aqueous solution; -■- = ΔE^{sol}. (b) Trends of the interaction energies between the central charged species and water molecules (ΔE^{X}, X = H_3O^+ or $H_5O_2^+$) with respect to the number of water molecules, obtained from B3LYP/TZVP calculations: -▲- = H_3O^+ in the gas phase; -△- = H_3O^+ in the continuum aqueous solution; -■- = $H_5O_2^+$ in the gas phase; -□- = $H_5O_2^+$ in continuum aqueous solution. —— = calculations without the counterpoise correction. - - - - - - = calculations with the counterpoise correction.

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

Additions and corrections can be viewed online by accessing the original article to which they apply.