Correction: Selective oxidation passing through $\eta^3$-ozone intermediates: applications to direct propene epoxidation using molecular oxygen oxidant

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The authors regret that the energetic spans for propene epoxidation over the Zr_NCCNO catalyst reported in Table 4 of the original article are incorrect. Additional calculations now indicate that an unwanted side reaction involving allylic H transfer makes the Zr_NCCNO catalyst ineffective for direct propene epoxidation. This finding affects the Abstract, Conclusions and Section 3.3.

In the sentence beginning “A new homogeneous Zr catalyst is designed…” within the abstract, the computed enthalpy energetic span should be changed from $\sim 28.3$ kcal mol$^{-1}$ to $\sim 74.6$ kcal mol$^{-1}$. This change also applies to the sentence beginning “The enthalpy energetic span of…” within Section 3.3 (page 27765). Furthermore, on the bottom row of Table 4, the values contributing to $E_{\text{span}}$: $(E)$, $(E_{\text{zp}})$, $(H)$ and $(G)$ should be changed from 28.4, 28.9, 28.3 and 41.6 kcal mol$^{-1}$, respectively, to 73.7, 76.2, 74.6 and 87.6 kcal mol$^{-1}$, respectively.

Further discussion on these data can be found in B. Yang and T. A. Manz, RSC Adv., 2015, 5, 12311–12322 and B. Yang and T. A. Manz, RSC Adv., 2016, 6, 88189–88215.

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