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CORRECTION

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Correction: Unravelling the impact of hydrocarbon structure on the fumarate addition mechanism – a gas-phase *ab initio* study

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Correction for 'Unravelling the impact of hydrocarbon structure on the fumarate addition mechanism – a gas-phase *ab initio* study' by Vivek S. Bharadwaj *et al.*, *Phys. Chem. Chem. Phys.*, 2015, **17**, 4054–4066.

In the case of toluene, our calculations indicate a small energy difference between the transition states of the *R* and *S* stereoisomers for the fumarate addition step. This arises due to the separate optimizations of the transition states and inherent uncertainties in the calculation (*cf.* Fig. 2 of the manuscript). This energy difference is translated into the reactant and product complexes due to the independent IRC calculations for each isomer. We expect that the energy difference between the two transition states for the stereoisomers in an unperturbed environment should be zero. However, this does not impact the results or the conclusions of the study, as evidenced by a re-evaluation of the kinetic model (Fig. 1) with this energy difference set to zero. The figure below compares the kinetic modelling results with the (original) small energy difference (left) and zero energy difference (right) in the transition states for the *R* and *S* stereoisomers of toluene.

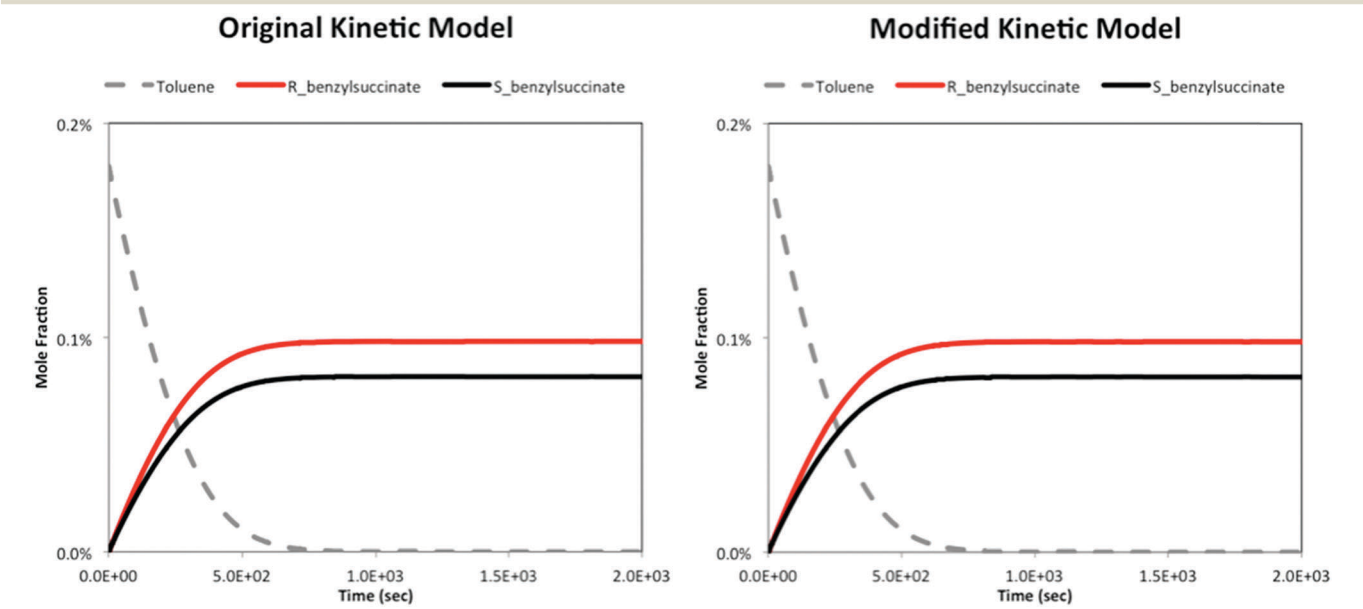

Fig. 1 Comparison of product distributions between the *R* and *S* isomers from the kinetic model with k_{-tst} values of 2.36×10^{-3} s^{-1} (left) and 4.82×10^{-4} s^{-1} (right) for the fumarate addition step. The other rate constant values are the same as those reported in Table 1 of the article.

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

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