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Correction: Kinetics and dynamics of the C(³P) + H₂O reaction on a full-dimensional accurate triplet state potential energy surface

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Correction for 'Kinetics and dynamics of the C(³P) + H₂O reaction on a full-dimensional accurate triplet state potential energy surface' by Jun Li *et al.*, *Phys. Chem. Chem. Phys.*, 2017, **19**, 23280–23288.

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We have discovered an inadvertent error in our code for computing the thermal rate coefficients by the quasi-classical trajectory (QCT) method. As a result, the corresponding QCT results in Fig. 6 of our original publication¹ were incorrect. The corrected QCT rate coefficients are now included in the new Fig. 6 below, which replaces the original Fig. 6. Reference 24 in the original publication is listed below as ref. 2. While the corrected QCT results are in less good agreement with the results from the canonical variational transition-state theory (CVT) with micro-canonical optimized multidimensional tunneling correction (μ OMT), both theoretical results are significantly lower than the experimental upper limit value. Thus, our original conclusions are not affected by this correction.

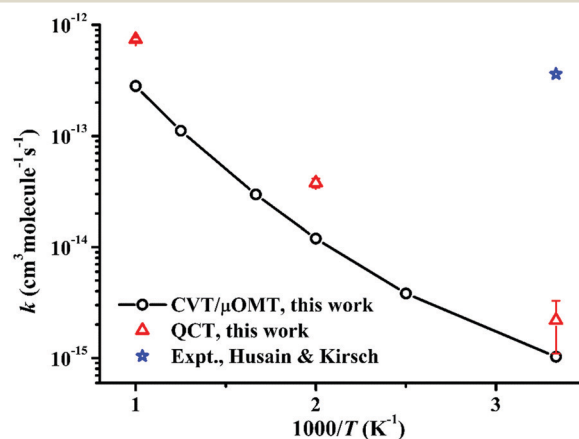


Fig. 6 Comparison of the CVT/ μ OMT and QCT rate coefficients (note the log scale) as a function of the inverse temperature. The experimental upper limit value of Husain and Kirsch² at room temperature is given for comparison.

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

References

- J. Li, C. Xie and H. Guo, *Phys. Chem. Chem. Phys.*, 2017, **19**, 23280–23288.
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