



Cite this: *Phys. Chem. Chem. Phys.*, 2020, 22, 4276

## Correction: Kinetics and dynamics of the C(<sup>3</sup>P) + H<sub>2</sub>O reaction on a full-dimensional accurate triplet state potential energy surface

Jun Li, \*<sup>a</sup> Changjian Xie <sup>b</sup> and Hua Guo <sup>b</sup>

DOI: 10.1039/d0cp90032j

Correction for 'Kinetics and dynamics of the C(<sup>3</sup>P) + H<sub>2</sub>O reaction on a full-dimensional accurate triplet state potential energy surface' by Jun Li *et al.*, *Phys. Chem. Chem. Phys.*, 2017, **19**, 23280–23288.

rsc.li/pccp

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 publication<sup>1</sup> 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 ( $\mu$ OMT), both theoretical results are significantly lower than the experimental upper limit value. Thus, our original conclusions are not affected by this correction.

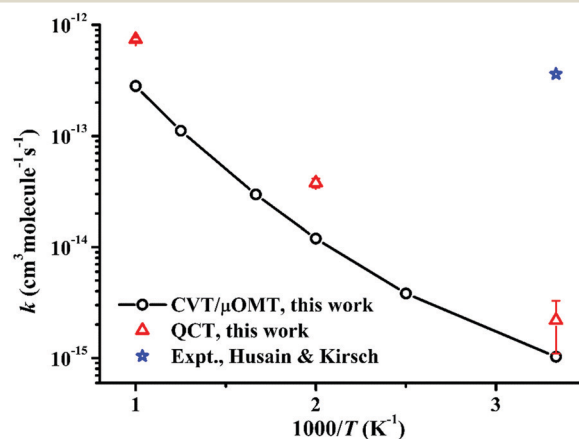


Fig. 6 Comparison of the CVT/ $\mu$ OMT and QCT rate coefficients (note the log scale) as a function of the inverse temperature. The experimental upper limit value of Husain and Kirsch<sup>2</sup> at room temperature is given for comparison.

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.
- D. Husain and L. J. Kirsch, *Trans. Faraday Soc.*, 1971, **67**, 2025.

<sup>a</sup> School of Chemistry and Chemical Engineering, Chongqing University, Chongqing 401331, China. E-mail: jli15@cqu.edu.cn

<sup>b</sup> Department of Chemistry and Chemical Biology, University of New Mexico, Albuquerque, New Mexico 87131, USA

