

# Evaluate the parametric uncertainty of RRKM/Master Equation rate constants

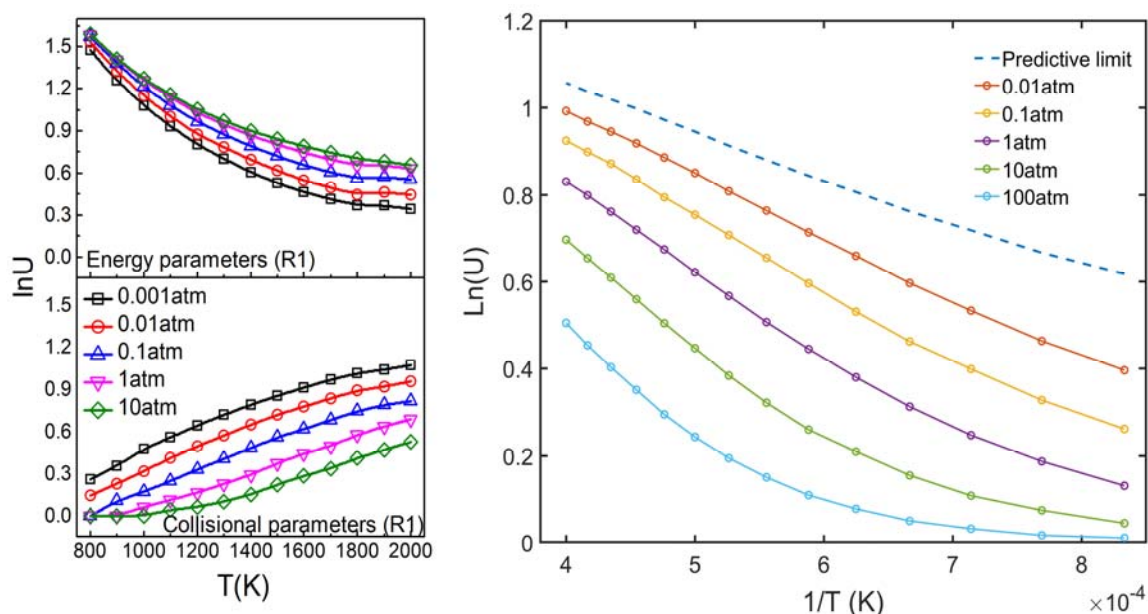
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The random sampling high dimensional model representation (RS-HDMR) method has been used to perform global uncertainty analysis for RRKM/Master Equation simulation [1,2]. Two conclusions have been made: 1. The second and higher order sensitivity is unimportant for uncertainty of RRKM/ME rate constants; 2. If the input parameters were divided into energy parameters, collisional parameters and frequency parameters, the partial uncertainties of computed rate constants monotonically increase or decrease with temperature and pressure, as shown in Fig. 1. Based on these conclusions, in the present work, we have extended the previous study to perform more rigorous uncertainty analysis on RRKM/ME rate constants aiming to quantitatively evaluate general rules for the temperature and pressure dependence of the uncertainties for computed rate constants. Figure 2 indicates that it might be possible to deduce partial uncertainty (uncertainties induced by collisional parameters shown in Fig.2) at any temperature and pressure if one knows the temperature and pressure dependent uncertainty of  $k$  at both high and low pressure limit. It should be noted that an artificial neural network (ANN) algorithm [3], which largely reduced the computational cost of uncertainty analysis, was used in this work.



## References

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- (2) Xing, L.-L.; Li, S.; Wang, Z.-H.; Yang, B.; Klippenstein, S. J.; Zhang, F., *Combust. Flame* **2015**, 162, 3427-3436.
- (3) Li, S.; Yang, B.; Qi, F., *Combust. Flame* **2016** (In Press)