Vibrational relaxation and recrossing effects in the $OH + SO \rightarrow H + SO_2$ reaction

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Synopsis Some details of the title reactions are presented in the frame of quai-classical dynamic studies

The understanding of elementary chemical steps in atmospheric acid rain formation is fundamental for mitigating its effects. It is believed the hydroxysulfinyl radical is an intermediate species for the production of atmospheric sulphuric acid. The present talk presents some discussions of a detailed quasi-classical trajectory study of the reaction between OH and SO radicals, considering both relaxation processes and recrossing effects [1, 2]. In the study, a global DMBE PES for the ground electronic state of the HSO₂ system was used. A discussion of kinetics and reaction pathways is also presented.



References

- [1] Garrido J D, Ellakkis S and Ballester M Y 2019 J. Phys. Chem. A 123 8994
- [2] Garrido J D, Ellakkis S and Ballester M Y 2020 Molecular Physics 118 e1751321

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