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The O + O_2 exchange reaction: symmetry, isotope effects, and influence of molecular forces

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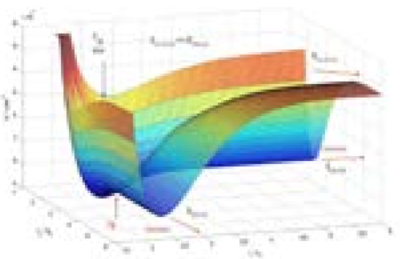
Statement of the Problem: Molecular oxygen O_2 is the most important molecule in Earth's atmosphere and stratospheric ozone O_3 protects us from 97% of UV radiations. The abundance in ^{16}O being 99.8%, O_2 and O_3 exclusively formed from it are dominant, thereby giving a reference for any process involving oxygen. A strong enrichment (about 10%) of O_3 in both ^{18}O and ^{17}O (the so-called mass-independent fractionation MIF), has first been observed decades ago. The three body recombination O + O_2 + M → O_3 + M is believed to be the main process leading to this enrichment and at low pressures, it can be partitioned into two steps: the formation of O_3 in a highly excited rovibrational state, from reaction O + O_2 → O_3*, and its subsequent stabilization by collision with an energy absorbing partner M (say N_2 or O_2), O_3* + M → O_3 + M. Thus, the efficiency of the exchange reaction O + O_2 → O_3* → O_2 + O, involving metastable O_3* as an intermediate, is one of the key parameters to understand ozone formation. This reaction is very fast and competes with the stabilization process.

Methodology: Using a newly developed, very accurate, potential energy surface (PES), we have realized computationally intensive full-quantum investigation of the dynamics of this process, using a time-independent formalism.

Results: We have, from first principles, computed reactive cross sections and reproduced measured rate constant for the ^{18}O + $^{32}O_2$ process, within experimental error bars. We will sum up resulting cross sections and rate constants for the various ^{16}O + $^{32}O_2$, ^{18}O + $^{32}O_2$, ^{17}O + $^{32}O_2$, ^{16}O + $^{36}O_2$ and ^{16}O + $^{34}O_2$ processes, discussing isotope effects and inclusion of permutation symmetry. We will discuss the strong influence of the PES.



Recent Publications

1. Dawes R, Lolur P, Li A, Jiang B, Guo H (2013) Communication: an accurate global potential energy surface for the ground electronic state of ozone. The Journal of Chemical Physics 139:201103-1-4.
2. Tyuterev V, Kochanov R, Campargue A, Kassi S, Mondelain D, Barbe A, Starikova E, DeBacker MR, Szalay PG, Tashkun S (2014) Does the 'reef structure' at the ozone transition state towards the dissociation exist? New insight from calculations and ultrasensitive spectroscopy experiments. Physical Review Letters 113:143002-1-4.
3. Guillon G, Honvault P (2016) Quantum dynamics of the ^{17}O + $^{32}O_2$ collision process. The Journal of Physical Chemistry A 120:8254-8258.
4. Guillon G, Honvault P (2017) Quantum dynamics of ^{16}O in collision with ortho- and para-$^{17}O^{17}O$. Chemical Physics Letters 689:62-67.
5. Rao TR, Guillon G, Mahapatra S, Honvault P (2015) Huge quantum symmetry effect in the O + O_2 exchange reaction. The Journal of Physical Chemistry Letters 6:633-636.
6. Rao TR, Guillon G, Mahapatra S, Honvault P (2015) Quantum dynamics of the ^{16}O+$^{36}O_2$ and ^{18}O+$^{32}O_2$ reactions. The Journal of Chemical Physics 142:174311-1-4.

Biography

Gregoire Guillon has his expertise in quantum scattering, inelastic and reactive, as well as in quantum Monte Carlo simulations. After working for several years in low temperature physics (cold molecules, helium droplets and hydrogen clusters), his latest results involve reactive processes occurring in an atmospheric chemistry context, as they are related to the ozone formation problem in stratosphere. He, together with PH, RC and VT has built this model after years of experience in research in laboratories worldwide.

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