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Quantum dynamics of the O+OH reaction: from ultracold collisions to astrochemistry[1] BALAKRISHNAN NADUVALATH, University of Nevada Las Vegas, Las Vegas, NV 89154, GOULVEN QUÉMÉNER, University of Colorado, JILA, Boulder, CO 80309, BRIAN KENDRICK, Theoretical Division, LANL, Los Alamos, NM 87545 — We present quantum dynamics of the O+OH→ H+O_2 reaction at temperatures ranging from the ultracold limit to astrophysically relevant values. Two different potential energy surfaces for the HO_2 system are employed in the calculations and the sensitivity of the rate coefficients to the details of the interaction potential is explored. The zero-temperature limiting value of the rate coefficient is predicted to be about 6×10^{-12} cm^3 s^{-1} [1], a value comparable to that of barrierless alkali metal atom - dimer systems. It is found that the rate coefficient remains largely constant in the astrophysically relevant temperature range 10 – 39 K [2], in agreement with the conclusions of a recent experimental study [3]. Implications of our findings to oxygen chemistry in the interstellar medium are discussed.
References: [1] Quéméner et al., arXiv:0811.4377v1 (accepted in Phys. Rev. A); [2] G. Quéméner, N. Balakrishnan, and B. K. Kendrick, J. Chem. Phys. **129**, 224309 (2008); [3] Carty et al., J. Phys. Chem. A **110**, 3101 (2006).

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