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Quantum reaction dynamics of ultracold O + OH collisions BRIAN KENDRICK, Los Alamos National Laboratory, JISHA HAZRA, Univerity of Nevada Las Vegas, GAGAN PRADHAN, NADUVALATH BALAKRISHNAN, University of Nevada Las Vegas — Quantum scattering calculations of the O + OH($v = 0$, $j = 0$) $\rightarrow$ H + O_2($v' = 0 - 3$, j') reaction are presented for the electronically adiabatic ground state $^2A''$ potential energy surface of HO_2. A numerically exact three-dimensional time-independent scattering method based on hyperspherical coordinates is used to compute rotationally resolved reaction probabilities, cross sections, and non-thermal rate coefficients. Total and vibrationally resolved scattering results are also presented. The scattering calculations span a wide range of collision energies between ultra-cold (1.16 μK) and thermal (298 K) and include several values of total total angular momentum $J = 0 - 3$. Interesting enhancements in the ultra-cold cross sections are observed for many of the transitions which are attributed to the presence of quantum resonances associated with the HO_2 complex.

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