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The following article "Dynamics of Hyperthermal Collisions of O(³P) with CO" appeared in American Chemical Society, Journal of Physical Chemistry A, Vol. 112 (11) (2008) and may be found at: <http://pubs.acs.org/>.

Abstract

The dynamics of O(³P) + CO collisions at a hyperthermal collision energy of 83 kcal mol⁻¹ have been studied with a crossed molecular beams experiment and with quasiclassical trajectory calculations on computed potential energy surfaces. In the experiment, a rotatable mass spectrometer detector was used to monitor inelastically and reactively scattered products as a function of velocity and scattering angle. From these data, center-of-mass (c.m.) translational energy and angular distributions were derived for the inelastic and reactive channels. Isotopically labeled C¹⁸O was used to distinguish the reactive channel (¹⁶O + C¹⁸O → ¹⁶OC + ¹⁸O) from the inelastic channel (¹⁶O + C¹⁸O → ¹⁶O + C¹⁸O). The reactive ¹⁶OC molecules scattered predominantly in the forward direction—i.e., in the same direction as the velocity vector of the reagent O atoms in the c.m. frame. The c.m. translational energy distribution of the reactively scattered ¹⁶OC and ¹⁸O was very broad, indicating that ¹⁶OC is formed with a wide range of internal energies, with an average internal excitation of 60 percent of the available energy. The c.m. translational energy distribution of the inelastically scattered C¹⁸O and ¹⁶O products indicated that an average of 15 percent of the collision energy went into internal excitation of C¹⁸O, although a small fraction of the collisions transferred nearly all the collision energy into internal excitation of C¹⁸O. The theoretical calculations, which extend previously published results on this system, predict c.m. translational and angular distributions that are in near quantitative agreement with the experimentally derived distributions. The theoretical calculations, thus validated by the experimental results, have been used to derive internal state distributions of scattered CO products and to probe in detail the interactions that lead to the observed dynamical behavior.