ACTIVATIONLESS REACTION OF NH (X $^3\Sigma^-$) AND O_2 IN SOLID Xe: FORMATION AND INFRARED SPECTRUM OF HNOO

SANDRA L. LAURSEN and JAMES E. GRACE, JR., Department of Chemistry, Kalamazoo College, Kalamazoo MI 49006.

The activationless reaction of ground-state NH (X ${}^{3}\Sigma^{-}$) with molecular oxygen is studied by annealing a solid Xe matrix containing O_{2} and trapped NH radicals formed upon UV photolysis of HN_{3} . The infrared absorptions which appear during this process are assigned to imine peroxide, HNOO, a new intermediate. Upon further long-wavelength photolysis, imine peroxide is destroyed, isomerizing to nitrous acid, HONO. Some features of the potential energy surface of this molecule are elucidated and are found to be in good qualitative agreement with published ab initio calculations.