PRODUCT BRANCHING RATIOS OF THE REACTION OF CO WITH H_3^+ AND ITS ISOTOPOMERS

HUA-GEN YU, *Department of Chemistry, Brookhaven National Laboratory, Upton, NY 11973.*

The reaction of CO with H_3^+, H_2D^+ and HD_2^+ has been studied using a direct *ab initio* molecular dynamics method, where the energies and forces used in trajectory propagations are determined by a SAC (scaling all correlation)-MP2/cc-pVTZ theory. For the H_3^+ + CO reaction, there are two product channels: (H_2 + HCO^+) and (H_2 + HOC^+). At room temperature, the thermal rate coefficient is predicted to be 1.37×10^{-9} cm^3.$molecule^{-1}$.s^{-1} with a product branching ratio [HOC^+]/[HCO^+]=0.28. In addition, dynamics results for the CO + H_2D^+/HD_2^+ reactions will also be reported.