

MQM 2022 Meeting – An Examination of the Reaction HOBr + H

Halogen containing species have been the focus of many atmospheric chemistry studies since the 1970s due to their ability to deplete the ozone layer. High level theoretical studies of fundamental halogenous reactions aid in understanding halogen cycles and their impact on the atmosphere. A particular reaction of interest involves hypobromous acid (HOBr) and the hydrogen radical (H). The present work examines three possible product channels of this reaction, HBr + OH (P1), BrO + H₂ (P2), and Br + H₂O (P3) at CCSD(T)/cc-pVQZ-PP//CCSD(T)/cc-pVDZ-PP. Work thus far has shown small barriers to transition states, 0.17, 11.16, and 3.95 kcal mol⁻¹ for P1, P2 and P3 respectively, as well as large exothermicity in the products, -38.04, -5.07, -65.93 kcal mol⁻¹ respectively.