Available online at **www.joac.info**

ISSN: 2278-1862

Journal of Applicable Chemistry, 2012, 1 (3):453-459

(International Peer Reviewed Journal)

Theoretical investigation study of Bromine radical reaction with ozone in stratospheric layer

Aqeel A-Hussein, and Abbas A-Ali Drea*

* Chemistry Department, College of Science, Babylon University, Hilla, IRAQ
Email: aadreab@yahoo.com

Received on 10th July and finalized on 28th July 2012

ABSTRACT

Theoretical study has been carried out to investigate the mechanism of reaction for bromine radical with ozone that's performed through PM3 of semi-empirical method. Geometry optimization and single point calculation through PM3-configuration interaction microstate have been done for all components of the suggested reaction and their transition states, in addition to vibrational analysis.The reaction of bromine radical with ozone is exothermic and spontaneously in the view of thermodynamic aspect. The energy barrier for this reaction is 3.9 kCal mol^{-1} *through TS1, while is 3.76 kCal* mol^{-1} *through TS4. Thermodynamic functions of activation* $\Delta H^* < 0$, $\Delta G^* < 0$ *and* $\Delta S^* < 0$ *,that is indicated the proceding of transition states are exothermic and spontaneous in gas phase at 298.15 K. The rate constant through TS1 equal to* $k_{TS1} = 3.09\times10^{9}$ *and* $A_{TS1} = 1.413\times10^{12}$ $mol^{-1}dm^3s^{-1}$ *at STP. While through TS4 equal to* $k_{TS4} = 2.73\times10^{10}$ *and* $A_{TS4} = 1.209\times10^{13}$ $mol^{-1}dm^3s^{-1}$ *at STP.*

Keywords: Bromine radical, ozone, potential energy surface, semi-empirical, and PM3.
