Study of Ozone Depletion by Halon-2402 in Stratospheric Layer Using Quantum Calculation Methods

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ABSTRACT

Structural properties of ozone and Halon-2402(1,2-dibromotetrafluoroethane) have been calculated using quantum methods likes DFT, ab-initio and semi-empirical (implemented in Hyperchem package 8.0) .Examination of bond reactivity for reaction component have been determined according to MP2//6-31G**(p,d) level of theories. Molecular orbital and their energy gap has been calculated using B3LYP//6-31G(d) and B3LYP//3-21++G**(p,d) level and parameter of bonds by ROHF//6-31G**(p,d) level. Values of rate constant and the reaction energy barrier were determine for all free radical reactions using MP2//3-21G**(2spd) level of theory. Steady state approximation method has been used to estimate the rate law of the depletion reaction.

It was found that the energy gap of ozone and Halon-2402 is 90.23 and 163 kCal/mol respectively. Photolysis reaction of Halon-2402 occurs through C-Br bond by 92.3 kCal/mol (309.95 nm)of light energy. The reaction of bromine radical with ozone is spontaneous and exothermic with energy barrier equal to 0.044 kCal/mol and rate constant equal to 3×10^{13} mol^{-1}dm^{3}s^{-1} , A= 2.33×10^{13} at STP. The mechanism of ozone depletion produced alkoxy radical by consuming four moles of ozone.

Keywords: Halone-2402, photolysis, Ozone depletion, Radical, potential energy surface, bond dissociation energy, MP2, B3LYP, and PM3.

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