IN THE NAME OF GOD

# A THEORETICAL STUDY ON THE REACTION OF OZONE WITH DOUBLE BOND.

BY

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*Dedicated to:*

**All honest people**

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## ABSTRACT

A Theoretical Study on the Reaction of Ozone with Double Bond

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In this work, the mechanism of ozonolysis reaction is reached by semiempirical (AM1 method) and ab initio methods (HF/6-31G(d,p),...). The minimum energy paths and the energy barriers for all steps of this reaction are reported.

The reaction contains several bimolecular and unimolecular steps. For each step, the rate constants and other kinetic parameters are calculated.

For bimolecular steps, the modified collision theory (by using Pacey's paper), are used. In this method, it is needed to calculate electronic partition function for the reactants and transition states, especially electronic degeneracy for these species. For this purpose, it is applied the correlation diagrams and electronic structures.

For unimolecular steps, the RRKM calculations are used. In this method, the rate constants are computed at different temperatures and pressures.

The ozonolysis reaction occurs in gas and liquid phases. In the gas phase, the reaction considered being non-equilibrium state, but in the liquid phase, considered being equilibrium state. For each case, the rate constant equations are considered.

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