

## Dissociation of cyclopropanone molecule and ion

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**Abstract.** Investigate the dissociation and ionization process of cyclopropanone molecules by using the Density functional method. Find the transition states of cyclopropanone molecule and ion, and get the products from transition state to isomer. In the same time, calculate frequency and energy. Confirm their transition states between the reactants and resultants through the Intrinsic Reaction Coordinates (IRC) calculation.

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**Key words:** density functional theory, cyclopropanone molecule, dissociation, ionization

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### 1 Introduction

Ketene is the main component of antimicrobial agents. The study on the properties of cyclopropanone is beneficial to refine new drug ingredients. Cyclopropanone compound is very unstable and research reports about cyclopropanone are not so many at domestic and abroad. As early as 1966, cyclopropanone was formed successfully by Hammond and DeBoer [1, 2] using ketene and diazomethane in Fluorine chloroform. In 2007, Ai *et al.* [3] reported that cyclopropanone could reach the excited states S1 in 292 ~ 365 nm wavelength light then  $\alpha$  C-C bond broke up. There is an intersection (TS1) between the ground state and first excited state on the fragmentation pathway of  $\alpha$  C-C bond. Then another C - C bond broke up and produced carbon monoxide and ethylene. Those are based on quantum chemical method using CASSCF B3LYP and MP2 in theoretically and experimentally. The report is described by the change of bond length and bond angle. And the reported results also provide some clues and bases on the further theoretical and experimental work on the dissociation of cyclopropanone molecule and ion.

In this paper, both cyclopropanone molecule and ion are described [4, 5]. We try to find the characteristics of the cyclopropanone molecule and ion by investigating the dissociation process. Some helpful information can be obtained, including the disabled

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process of cyclopropanone molecule and ion from its potential energy surface. Therefore, it is significant for us to work on the dissociation of potential energy surface. Here, two possible dissociation paths on molecule are reported. One possible dissociation path is that the 2C - 4C single bond breaks up and forms an open-loop structure, then another 2C - 3C bond breaks up and produces CO and C<sub>2</sub>H<sub>4</sub>. The other is that 3C - 4C bond breaks up and forms isomer, then dissociates C<sub>2</sub>H<sub>2</sub>O and CH<sub>2</sub>. It is found that the configuration of the cyclopropanone ion is unstable, and the open-loop structure of stable ion configurations is got.

## 2 Basic theory and computational methods

Quantum mechanics theory is the basic theory in microscopic field, in which all phenomena can be explained with knowledges of quantum mechanics. Therefore, we use modern methods of quantum chemistry and atomic molecular theory to study the molecular problems [6]. Density functional theory is a powerful computational tool to calculate the larger molecules systems. Compared with Hartree-Fock (HF) and Moller-Plesset (MP), it can save much time. In this work, geometrical parameters of the reactants, products, intermediates, and transition states are optimized basing on the unrestricted B3LYP [7] with the 6-31 + G (d, p) basis set from density functional theory (DFT). Harmonic vibration frequencies that are calculated at the same level are used for the characterization of stationary points. Meanwhile, according to further analysis by IRC calculations [8-10], the transition states are between reactants and products. All calculations are performed using GAUSSIAN 03 programs.

## 3 Results and discussion

Cyclopropanone formula is C<sub>3</sub>H<sub>4</sub>O. By optimizing structures and correcting correlation energies of the molecule, the energy is -191. 8966 Hartree, and there is no imaginary frequency. The optimized geometry of stationary point has been plotted in Fig. 1. The vibration frequencies and the relative intensities are listed in Table 1 and showed in Fig. 1. There are many vibrational modes around the vibration peaks. From Table 1, the maximum vibration intensity of 358.371 KM/Mole occurs at the frequency of 1930.79 cm<sup>-1</sup>, its intensity is 108.244 KM/Mole at the frequency of 964.151 cm<sup>-1</sup>, and its intensity is 27KM/Mole at the frequency of 1018.02 cm<sup>-1</sup>. In addition, its intensity is 15 KM/Mole at the frequency of 1072.33 cm<sup>-1</sup>. Analysis on a few frequencies is given as follows while other modes are neglected.

First, from Table 1, at the frequency of 1930.79 cm<sup>-1</sup> and intensity of 358.371 KM/Mole, 1 O atom and 2 C atoms have the strongest vibration. It should make 2C - 3 C bond or 2C - 4 C bond break up, forming the products of CO and C<sub>2</sub>H<sub>4</sub>, or it may make O - 2 C bond break up, forming O and C<sub>3</sub>H<sub>4</sub>. However, transition states of these two dissociations are not found [11], which shows they are difficult to happen! So it is possible that it makes