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Study of Electronic Effect in Organic Reactions Introduction

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ABSTRACT. *In the fields of chemistry, chemical engineering, and even materials, organic reactions have always been an important part of research and actual production due to their special characteristics. In organic reactions, the electronic effect and steric hindrance effect are very important to the stability of organic compounds, especially in the electrophilic addition of carbon carbon heavy bonds and the deactivation of single substituted aromatic compounds, the accurate analysis of related electronic effects can always solve the problem. Therefore, this paper aims to explore the essential mechanism of electronic effects in organic reactions, in order to solve practical problems in actual chemical production and chemical research.*

KEYWORDS: *Electronic effect, Induced effect, Conjugate effect, Electron cloud density*

1. Introduction

The electronic effect mentioned in this paper mainly refers to two kinds: induction effect and conjugation effect. In most cases, when studying organic reactions and related chemical applications, it is customary to analyze the inducing effect and conjugate effect separately. Moreover, because the action intensity of the two effects is different in different types of organic substances, the analysis process is complicated because it must be judged together with the related properties of substances.

At present, the author found a method that can simplify the judgment of electronic effect, that is, to directly judge the charge density and electron cloud density distribution without thinking about ± I effect and ± C effect.

2. The Essence of Electronic Effect in Organic Reaction

Electronic effects can be roughly divided into two categories, namely, induced effects and conjugate effects. Because of their special characteristics, super-conjugate effects are not analyzed here, and will be listed separately later. The induction effect can be divided into electron-donating induction effect (+I) and electron-withdrawing induction effect (-I), i.e. the phenomenon that bonding electrons shift along the atomic chain due to their different polarities (electronegativity). The conjugation effect can be divided into two kinds: the electron donating conjugation effect (+ C) and the electron absorbing conjugation effect (- C), that is, the average distribution (delocalization effect) of π electron and P electron of atom, and the bond length tends to average, that is to say, the energy of the system is lower and more stable. Such as the analysis of the different stability of cis-trans isomers in different double bond compounds [5].

In organic reactions, the reaction process and products are affected and regulated by electronic effects. In essence, the change of electronic cloud density distribution causes the change of material properties, which indirectly affects the process of organic reactions.

2.1 Induction Effect

Induction effect means that the different polarities (electronegativity) in the molecule or atomic group cause the bonding electrons to move along the atomic chain, generating positive and negative charge centers, so that the next reaction can proceed.

Because it only involves the change of the electron cloud density distribution, which causes the change of the bond polarity, it does not cause the charge transfer and valence state of the whole system to change. Therefore, the electrostatic effect rapidly weakens from near to far along the atomic chain, exists in the local range of the system, can be superposed to a certain extent, and has additivity.

2.2 Conjugate Effect

The conjugation effect is that the change of π electron and P electron (or π electron and π electron) distribution in the system results in the flattening of the bond length and the decrease of the energy of the system.

The conjugate effect often requires the following two points: first, the related atoms are coplanar, and each atom provides a p-orbit (or suitable d orbit) in the same direction; Double the number [4].

2.3 The Sum of the Two Effects

Under normal circumstances, the analysis of an organic substance is based on the combined analysis and consideration of induction effect and conjugation effect. After consulting, there are also thinking about the method of dipole moment correlation calculation [3], but because there are usually induced dipoles in organic reactions [4], it is not conducive to the promotion of the concept, that is, beyond two kinds of electronic effects, to analyze directly in the thinking of electronic cloud theory.

3. Theoretical Thinking

3.1 Electronegativity Correlation

The induction effect is mainly determined by the electronegativity of atoms, so theoretically the electron bias must be closely related to the electronegativity between the two atoms. On the data, the electronegativity is a corresponding scale established by Pauling with the fluorine element as 4.0, so an equivalent structure can be taken to obtain an accurate result.

In most cases, carbon will still show different electronegativity under different hybrid and carbon ion situations [6]: It is generally believed that compounds are composed of atoms and chemical bonds, and different chemical bonds have different bond lengths, which is also determined by electronegativity. According to the theory of electron cloud, the electron pair bias can be regarded as a point in the bond line, which can be calculated from the bond length and electronegativity. Among them, the difference Δ I between the effective carbon chain length NC and the induced effect index I was correlated [1], so the author was inspired by it and chose a more understandable method to replace it.

Such as:

$$D = L\frac{EN_i}{EN_0 + EN_i}$$

(L-Bond length EN0-Central atom electronegativity ENi-iAtomic electronegativity)

The theoretical point (hereinafter referred to as P) can be obtained from the ratio of electronegativity, and a theoretical value d without real meaning can be obtained on the point P.

From a molecular point of view, the key lies in the selection of the central atom (of course, organic molecules often choose C atom). After obtaining the P points of each bond, the connection line from the central atom to each P point takes D value as the module length to obtain different vectors. Add all the vectors to get a final theoretical point (called P '), which is the negative electric center (δ-) of this molecule, and the positive electric center (δ +).

Then take the position of the central atom as O, and calculate the total negative charge center (δ-) P with the bond P point (Pi) by the following formula:

$$\overrightarrow{OP} = \sum_{i} \overrightarrow{OP_i}$$

3.2 For Example

1) 4. C= o Common Bond Length143pm

2) 5. C≡n Common Bond Length115.8pm
3) 6. C-h Common Bond Length106pm
4) 7. O-h Common Bond Length264pm
5) 8. C-C Common Bond Length154pm(Center 77pm)

Electronegativity C (2.55), O (3.52), N (3.04), H (2.09), namely P1 point is 83.4pm from C atom, P2 point is 62..4pm from C atom, P3 point is 47.7pm from C atom The P4 point is 98.4pm from the O atom.

Application example:

The “P” point of formaldehyde lies on the carbon oxygen bond and is 35.7 PM away from the carbon atom. The “P” point of vinyl nitrile is located on the carbon carbon single bond and is 154 - (77 + p3-p2) = 91.7pm away from the carbon atom connecting the cyano group.

4. Inspiration and Prospect

The decisive effect of electron cloud density distribution on electron effect gives us a new way to judge the organic reaction process and products. This method seems to be more complicated. In fact, it partially solves the difficult point of the concept of positive and negative electrical centers. In addition, it solves the problem that three-dimensional molecules cannot easily determine the position of the positive and negative electrical centers due to induced effects. It has high efficiency.

However, there are some problems in understanding and implementation, such as more complex data and more front-end steps. On the one hand, how to calculate the density distribution of electron cloud by means of physical modeling and mathematical demonstration. Studies have shown that the electron cloud density distribution has a great impact on organic reactions, and the change in the electron cloud density distribution has a decisive effect on the reaction history and the products generated. Therefore, a question is raised: Whether the density distribution of electron cloud can be obtained by mathematical demonstration and physical modeling calculation, and then the organic reaction can be deduced according to its distribution change, and then the organic reaction can be accurately predicted.

On the other hand, the change of electron cloud density distribution is regulated by the organic reaction. The reverse direction in the organic reaction process affects the electron cloud density distribution, thus changing it and then pushing the organic reaction forward. Therefore, whether there is a simpler calculation model to reveal the two-way relationship between the change in the density distribution of the electron cloud and the organic reaction will become a challenge worth exploring in the field of organic reaction mechanism.

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