ANALYSIS OF INSULATING CHARACTERISTICS OF SF_6 AND CF_3I FROM THE POINT OF VIEW OF MICROSCOPIC FEATURES

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ABSTRACT

Sulphur hexafluoride (SF_6) has been specified as a greenhouse gas. The root causes of the great insulating performance of SF_6 such as microscopic structure are still worth studying to find other alternative insulating gases. Many researches of trifluoroiodomethane (CF_3I) have shown that CF_3I has many excellent properties which make it one of the possible alternatives of SF_6. In this paper we attempted to explore part of the microscopic reasons for their insulating properties. We started research from atomic and molecular physics features such as atom compositions, molecular structures and covalent bonds of some organic insulating gases to expound the significant relationships between molecular properties and electron attachment processes. For the same list of molecular features we compared SF_6 and CF_3I to get the necessary microscopic features as basic condition which can be used in the pre-analysis of insulating performance for new gases. Additionally, it can also be used to research gas mixtures for insulating characteristics complements from the point of view of microscopic properties.

1. INTRODUCTION

Sulphur hexafluoride (SF_6) is widely used in gas-insulated power equipment, but due to its high global warming potential (GWP) which is 23900 times greater than that of CO_2, SF_6 has been specified as a greenhouse gas and proposed restrictions on the use in Kyoto Protocol [1]. Therefore the environment problems and the costs of the usage of SF_6 are all growing. Many scholars have focused on the study of alternative gases. Because of the excellent insulating and arc performance, to find a perfect alternative gas which can meet all the electrical requirements as SF_6 is a complex work [2].

Some scholars test the insulation properties of various gases and gas mixtures by experiments. Through the experiments several gases and mixtures have been concerned such as high pressure N_2, CO_2, trifluoroiodomethane (CF_3I) and the mixtures of SF_6 with N_2 and CO_2 [3-8]. They all have a lower GWP than SF_6 and almost the same level of insulating performance. So far we have not found a perfect substitute gas which can be applied in all the electrical equipment to replace SF_6 yet. To find a perfect substitute solution requires a systematic study of the insulating performance of SF_6 and its nature reason. The study from the microscopic point of view may lead a deeper understanding of the relationship between molecule structure and insulation which can be helpful to find potential alternative [9, 10].

The gas insulation is actually to limit the free electrons and the electron flow as a barrier. That is to say insulting gas should lead the reducing of electron movement and avalanche process as well. The gas molecules and free electrons may have several processes during the insulation including the electron collision ionization processes, electron attachment processes, electron diffraction processes and interruption processes [11]. To achieve this limit effect, electron attachment processes are important to reduce the electron density. Experiments show that lots of electronegative gases which have good insulating properties contain halogen elements such as fluorine, chlorine or iodine.

On the other hand, the electron-attachment capacity depends not only on the elements of insulating gas, but also has a great relationship with the atomic structure of the molecular orbits. J. C. Devins tested many gases for their dielectric

strength especially some organic gases [12]. As the tests shows, besides the greater molecule size which can increase the effect of blocking electrons, the insulating performance present a regular change between the gas and the dielectric strength of the types of molecules. For example, ethane (C_2H_6) and ethylene (C_2H_4) have same elements and similar molecule structures. But in A. E. D. Heylen and T. J. Lewis' tests C_2H_4 has an almost 1.6 times dielectric strength than C_2H_6. Double bonds in organic gases can have a significant impact on the insulation performance of the gas [13]. Double bonds may provide more easily attached molecular orbits to free electrons [14]. This effect is similar to the electronegative gas molecules which have halogen elements. Therefore, the attachment of free electrons is the process to provide lower energy level molecular orbits for electrons. That impact indicates a set microscopic feature of insulating gases. Two aspects features of gas molecules will be helpful:

- Unoccupied molecular orbits in low energy level for the gas molecule
- Occupied molecular orbits in low energy level for the negative ion of gas molecule and electron

In the rest of this paper we study from the relationship between electron-attachment capacity and microscopic structure by calculating the molecule unoccupied molecular orbits of C_2H_6, C_2H_4 and other organic gases which are listed in section 3. And then verify the insulating impact of molecular orbits with the compare between SF_6 and the potential substitute gas CF_3I in section 3. Afterwards we briefly present a conclusion of molecular orbits' impact to insulting performance and suggestions for future microscopic work.

2. METHODS

We have calculated the lowest unoccupied molecular orbits (LUMO) with parametric model 3 (PM3) semi-empirical method [10, 15]. This method bases on neglecting of diatomic differential overlap. That is to say this semi-empirical method will neglect certain electron-electron interactions. We use PM3 method to build the molecule structure model and calculate alpha orbits of selected molecules both occupied and unoccupied. To verify whether the molecules are stable after the electron attachments, we also calculate the negative ions' orbit energy of gas molecules. We focused on the highest occupied molecular orbit (HOMO) of the negative ion. This method has been used to check whether the reactions can occur. It also can show how many unoccupied molecular orbits the gas molecule have with the similar low energy level.

For the molecules, due to they are electrically neutral, the spin multiplicity of molecule is 1. For the negative ion the total charge is -1 and the spin multiplicity is 2. As during the electron collision processes, the gas molecules may re-form a new molecule or ion, this paper only analyse the situation with a free electron attachment [16].

3. RESULTS AND DISCUSSION

We first present the molecular orbits result of C_2H_6, C_2H_4 and acetylene (C_2H_2) in Table. 1. Due to their flammability they all can't be applied as insulating gas. But the regular change of insulating performance between them is meaningful.

From the results we can easily find the lowest unoccupied molecular orbits energy of C_2H_4 and C_2H_2 are significantly lower than C_2H_6. That means free electrons can be easier attached by the gas molecules. The molecule structure differences between them are the covalent of carbon atoms. C_2H_2 molecules have a triple bond and C_2H_4 molecules have a double bond. For example, C_2H_4 has a sigma-bond and a pi-bond. Both bonds also have an unoccupied anti-bond. For the free electrons the unoccupied anti-bond have a lower energy level orbit which make it easier to occur attachment processes than the orbit of sigma-bond. These structure differences lead the different insulting performances.

Table. 1 Molecular orbits Energy of C_2H_6, C_2H_4 and C_2H_2

	Lowest unoccupied molecular orbits (eV)	*Second lowest unoccupied molecular orbits (eV)*	*Highest occupied molecular orbit (eV)*
C_2H_6	17.947	17.952	-12.519
C_2H_4	8.0803	17.946	-8.2280
C_2H_2	10.786	10.786	-9.5205

Table. 2 Negative Ion Orbits Energy of C_2H_6, C_2H_4 and C_2H_2

	Lowest unoccupied molecular orbits (eV)	*Highest occupied molecular orbits (eV)*	*Second Highest occupied molecular orbit (eV)*
C_2H_6 + e	27.619	14.805	-0.6955
C_2H_4 + e	20.335	6.0305	3.6660
C_2H_2 + e	22.268	9.4406	3.5064

C_2H_2 and C_2H_4 have the smaller molecule size than C_2H_6 but have greater dielectric strength. The calculate results of molecular orbit energies show consistency with the result of A. E. D. Heylen and T. J. Lewis. That means the suit style of covalent bond can lead the improvement of insulation by change the orbits energy. The unoccupied orbits energy has a great impact with the insulation.

Table. 2 shows the negative ion orbits energy of C_2H_6, C_2H_4 and C_2H_2 after the attachment processes. The lowest unoccupied molecular orbits energies are all higher which means the molecule hardly to absorb another free electron especially for C_2H_6. The second column listed the highest occupied molecular orbits energy of ions. The lower energy C_2H_4 and C_2H_2 have means the molecule can stay stable respectively. On the other hand, with the energy transport, other electrons and orbits have also been excited which make the ion system unstable. With a lower energy orbits, the electrons can also get lower energy after the ion decomposition.

After measuring the molecular orbit energy of organic gases and to get the great impact between molecular orbits energy and dielectric strength, we also calculate the orbit energy of SF_6 and the potential alternative CF_3I to check whether the unoccupied orbits energy is a significant reason for their insulating performances. Table. 3 shows the results.

Table. 3 Molecular orbits Energy of SF_6 and CF_3I

	Lowest unoccupied molecular orbits (eV)	*Second lowest unoccupied molecular orbits (eV)*	*Highest occupied molecular orbit (eV)*
SF_6	5.1239	8.5525	-9.5295
CF_3I	7.1346	15.054	-8.3460

Table. 4 Negative Ion Orbits Energy of SF_6 and CF_3I

	Lowest unoccupied molecular orbits (eV)	*Highest occupied molecular orbits (eV)*	*Second Highest occupied molecular orbit (eV)*
SF_6 + e	14.867	4.0754	-4.0430
CF_3I + e	18.449	0.24670	0.24670

As the Table. 3 shows SF_6 has an extremely low unoccupied molecular orbits energy. According to the impact to dielectric strength, the low energy unoccupied orbits of SF_6 provide excellent attachment ability. While CF_3I also has a respectively low energy orbits but the second and third lowest unoccupied molecular orbits are in the energy level about 15eV. That means the lowest orbit is benefit from the only one iodine atom. So the element composition leads a great ability of electron attachment. SF_6 and CF_3I both have a great advantage that the highest and the second highest occupied molecular orbits of their negative ion are still in a low level which can maintain the ion system in a respectively stable state. Most electrons haven't been excited during the attachment process like the organic gases have.

4. SUMMARY AND CONCLUSION

We have present two sets of molecular orbits energy of several insulating gases. The first set of data is about the organic gases. With the different molecule structure, the unoccupied molecular orbits energy shows consistency with the gas dielectric strength. The difference of orbits energy acts as a nature reason for the entirely different insulating performance between similar gases. In the second set of data we present that SF_6 and CF_3I both have the molecular orbits advantage for insulation. And these microscopic features are based on the halogen element.

Even molecular orbits energy impact the attachment process in some level, the insulation processes are also determined by many other feature including microscopic and macroscopic such as cross section, electric dipole moment. Molecules may decompose during the electron collision process, so the study about the orbits should also focus on the reaction products in the future work. But the work from the gases

molecules can lead a direct way to the nature reason of insulation. It is also necessary for finding or reforming the substitute insulation gases.

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