Conformation Analysis of Environmentally Friendly Insulating Gas C5-PFK

ZHICHENG LEI [ID], FUPING ZENG [ID], JU TANG, ZHAOFENG WAN [ID], MINGXUAN ZHANG, AND LIANGJUN DAI

School of Electrical Engineering and Automation, Wuhan University, Wuhan 430072, China

Corresponding author: Fuping Zeng (Fuping.Zeng@whu.edu.cn)

ABSTRACT The environmentally friendly insulating gas C5-PFK has the potential to replace SF_6 in medium and low voltage gas insulated electrical equipment due to its good environmental performance and insulation strength. However, since C5-PFK molecule has rotatable C–C single bonds, the geometry will change when collided with each other or obtained external energy, which may have an impact on the stability and reactivity of C5-PFK molecule. In this paper, the geometry of C5-PFK molecule is optimized by the density functional theory-B3LYP-D3(BJ) method under the triple-zeta polarization basis set and high convergence criterion. The two C–C bonds connected with the carbonyl group (–C = O–) in C5-PFK molecule are rotated to scan its potential energy surface. Then, we obtained four possible conformers that might exist in C5-PFK molecule. The molecule structure, molecule energy, Mayer bond order, and energy levels (HOMO, LUMO orbital included) of frontier molecular orbital were analyzed to study the four conformers' stability and reactivity, which will pave the way for follow-up research work such as thermostability, transition state, reaction pathways, and adsorption behavior of C5-PFK.

INDEX TERMS C5-PFK insulating gas, conformation analysis, stability, reactivity.

I. INTRODUCTION

With the continuous development of the power industry, the installation of gas-insulated equipment in the power grid system is getting larger, meanwhile, the use of SF_6 is also increasing rapidly. The process of commissioning, overhauling, leaking and recycling of SF_6 gas-insulated equipment will release SF_6 into the atmosphere [1]. The IPCC reported that SF_6 has the largest Global Warming Potential (GWP) value among the greenhouse gases, whose value of 500 years is 32,400. Due to the chemical stability of SF_6, the residence time in the atmosphere can be 3200 years long [2]. According to incomplete statistics, the SF_6 gas content in the atmosphere has increased by about 20% in the past five years, and nearly 80% of the globally produced SF_6 are used in the power industry [3], [4]. China is likely to become the largest SF_6 emitter by 2020 as no legal or voluntary agreement supports SF_6 emissions reductions while the country is likely to remain a large producer of equipment for transmission and distribution of electricity [2]. According to the United Nations Framework Convention on Climate Change-The Kyoto Protocol, which was enacted in Kyoto, Japan in 1997, clearly stipulated that SF_6 is one of the six greenhouse gases, and requires developed countries that are large emitters of greenhouse gases to take specific measures to limit greenhouse gas emissions [5]. The US, EU, UK and Japanese governments have all worked with power companies to propose a series of measures to reduce greenhouse gas emissions. California has proposed reducing the use of SF_6 in the electrical sector year by year from 2020. The EU plans to reduce SF_6 to 2/3 in 2014 by 2030 [6]. The content of SF_6 gas in the atmosphere increases at a rate of 8.7% per year. So far, SF_6 gas has accounted for more than 15% of the total greenhouse gas emissions [7], so it is urgent task to look for an environmentally friendly alternative to SF_6 as an insulating medium for electrical gas-insulated equipment for long-term environmental protection considerations [8].

At present, the exploration of new environmentally friendly insulating gas has become a research hotspot of scholars for more than a decade [4], [9], [10]. ABB Company put forward the application prospect of perfluoroketone insulating gas ($C_nF_{2n}O$) in electrical equipment. The C5-perfluoroketone insulating medium $C_5F_{10}O$ is non-combustible, non-explosive and non-toxic, and its GWP

The associate editor coordinating the review of this manuscript and approving it for publication was Wu-Shiung Feng.
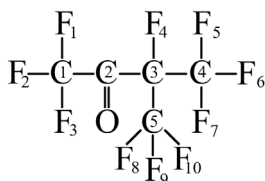
FIGURE 1. Chemical configuration of C5-PFK.

FIGURE 2. The trifluoromethyl group (CF_3·) in red and the heptafluoroisopropyl group (C_3F_7·) in green rotate 360° around the C-C single bond, respectively.

value is close to 1, the Ozone Depletion Potential (ODP) is 0, and the dielectric strength is about twice that of pure SF_6 gas [11], [12]. Although C5-PFK has excellent performance in insulation and environmental protection, its liquefaction temperature is as high as 26.9 °C. It cannot be used alone, which needs to be mixed with a low liquefaction temperature buffer gas such as CO_2, N_2, Air, etc. to prevent its liquefaction.

The structural formula of C5-PFK molecule is shown in Fig. 1 There are five carbon atoms in the molecule, and the carbonyl group (-C = O-) is bonded to the trifluoromethyl group (CF_3·) and the heptafluoroisopropyl group (C_3F_7·) at both ends. Because there are several C-C single bonds in the C5-PFK molecule structure, when the C5-PFK molecule is collided with each other or obtained external energy, the C-C single bond may rotate, which produces a different arrangement of each atom or group of the molecule in the space, that is the conformer for a molecule. Different conformers of C5-PFK molecule may exhibit different physical and chemical properties, or exhibits different reactivity during the reaction [13]–[19].

The molecule energy and structure of different conformers of C5-PFK molecule differ, which lead to the difference of required energy for decomposition during discharge or heating, and may also affect the transition state and decomposition pathway to some extent [20]–[22]. When C5-PFK molecule participates in the adsorption or chemical reactions on solid (metal materials or organic insulating material) surfaces, the C5-PFK conformers have different range of molecular frontier orbitals or adsorption site, which may influence the reaction mechanism between the gas-solid interface [23]–[25]. Therefore, conformation analysis of C5-PFK molecule has certain guiding significance for its further study.

II. METHODS

Quantum chemical calculation is a powerful tool for theoretical analysis of chemical reactions. Due to the superiority of Density Functional Theory (DFT) in terms of calculation amount and accuracy, it has been widely used in theoretical chemistry. The simulation research and analysis in this paper are carried out on the Amsterdam Modeling Suite (AMS). The ADF module is provided in the AMS platform [26]–[28], which can be used for the DFT calculation in aperiodic systems (molecules, clusters, etc.). Many previous studies [20], [29]–[33] have shown that, the exchange-correlation functionals Hybrid:B3LYP method is very suitable for the DFT calculating of C/O/F
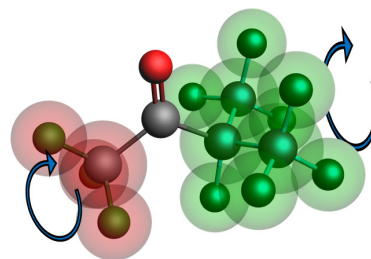
element system. Compared with other DFT methods, Hybrid:B3LYP has high precision and low computational cost simultaneously, and the obtained characteristics of the molecular ground state are approximate. It is generally accepted within the error range to calculate the optimized geometric data based on Hybrid:B3LYP method. Therefore, it is feasible to use the approximation to calculate other properties of the molecule and the chemical reaction of the system.

However, the calculated result for a system dominated by dispersion (such as physical adsorption, macromolecular conformation, weak polar molecular clusters, etc.) can not be described precisely using the Hybrid:B3LYP method. The most effective way to describe the dispersion effect is to introduce the empirical dispersion correction term DFT-D3 [34]. Later, Tao J found that the use of Becke-Johnson damping with a clearer physical meaning can make the results a little better, and the advantage of describing the intramolecular dispersion is more significant, that is often referred to as DFT-D3(BJ) [35].

In this paper, the molecule conformation analysis of environmentally friendly insulating gas C5-PFK was carried out to study the relationship between the geometry and energy of different conformers. Firstly, use Hybrid:B3LYP-D3(BJ) method, Triple-Zeta-P basis set and high convergence standard to optimize the geometry of C5-PFK molecules to obtain the most stable configuration which has the lowest energy. Secondly, the potential energy surface is scanned by rotating the dihedral on the C-C single bonds at both ends of the central carbonyl group (-C = O-). Thirdly, obtain the relatively stable C5-PFK conformers from the corresponding relationship between molecular energy and molecule structure. At last, study the Mayer bond order, energy-levels of frontier molecular orbital and molecule energy.

III. RESULTS

A. POTENTIAL ENERGY SURFACE SCAN

First, the F_1-C_1-C_2-O and F_4-C_3-C_2-O dihedrals, that is in the C-C single bonds at both ends of the central carbonyl group (-C = O-), are rotated to obtain the relationship between energy and dihedral of different molecule structures, as shown in Fig. 2. Since the bond lengths and angles of three C-F bond of the trifluoromethyl group (CF_3·) are nearly identical, the energy change curve approximately

periodically changes during the rotation of the F_1-C_1-C_2-O dihedral. The energy curve shows the three low points at about 120°, 0° and 120°, where one of the C-F bond of trifluoromethyl group ($CF_3\cdot$) is parallel to the carbonyl group (-C = O-), and the minimum energy is −4.1431 Hartree at about 0°.

At about −60°, 60°, and 180°, the energy curve shows three high points, and the maximum energy is −4.1380 Hartree at about −60°. Although the energy is low at −120° and 120°, the energy gradient is still high and not stable enough. During the rotation of trifluoromethyl group ($CF_3\cdot$), the most stable configuration with the lowest energy is at the position of the F_1-C_1-C_2-O dihedral equal to 0° since its lowest energy and energy gradient. The heptafluoroisopropyl group ($C_3F_7\cdot$) is not nearly as tetragonally symmetrical like the trifluoromethyl group ($CF_3\cdot$), but is approximately mirror-symmetric. Therefore, the energy and energy gradient curves in the figure are shown approximately symmetric about the F_4-C_3-C_2-O dihedral of 0°. It can be seen that C5-PFK molecule has an energy of −4.1432 Hartree at the F_4-C_3-C_2-O dihedral of about 180°, which is much lower than other configurations, and also appears two low points of −4.1376 Hartee.near −10° and 10°. The energy curve shows two high points of −4.1270 Hartree at −80° and 80°, respectively. Meanwhile, a small local high point appears at 0°, whose energy is −4.1369 Hartree. The energy gradient curve also appears two low points around 0° and 180°. Therefore, the C5-PFK molecule structure may not be stable enough when the F_4-C_3-C_2-O dihedral is 0°, somehow it will rotate to the −10°, 10° position to seek a more stable configuration.

The C5-PFK molecule structure generated by the rotation of the radical group around the C-C single bond can be mutually transformed. Only the stable molecule structures with locally lowest energy at the low points of the potential energy surface can be called conformers. From Fig. 3, we can see that, the energy change of the trifluoromethyl ($CF_3\cdot$) and heptafluoroisopropyl groups ($C_3F_7\cdot$) rotation around the C-C single bond in C5-PFK molecule exhibit a certain periodicity or symmetry. In order to reduce the simulation computation time, the F_1-C_1-C_2-O dihedral rotation range is from −60° to 60°, and the F_4-C_3-C_2-O rotation range is from 0° to 180° when scanning for the potential energy surface of C5-PFK molecule.

Four low points of energy are selected from the potential energy surface as shown in Fig. 4, where the corresponding molecule structures are intercepted, named C-0, C-1, C-2, C-3. The four molecule structures' frequency is scanned, whose results show that these vibration frequency of four configurations is all positive, so it can be judged that the configurations corresponding to C-0, C-1, C-2, C-3 is the stable point on the potential energy surface, that are four conformers of C5-PFK molecule. Table 1 gives the bond lengths and dihedrals and Fig. 5 shows the view of the C5-PFK conformer along the three axes of X, Y and Z. C-0 conformer is the most stable configuration with lowest
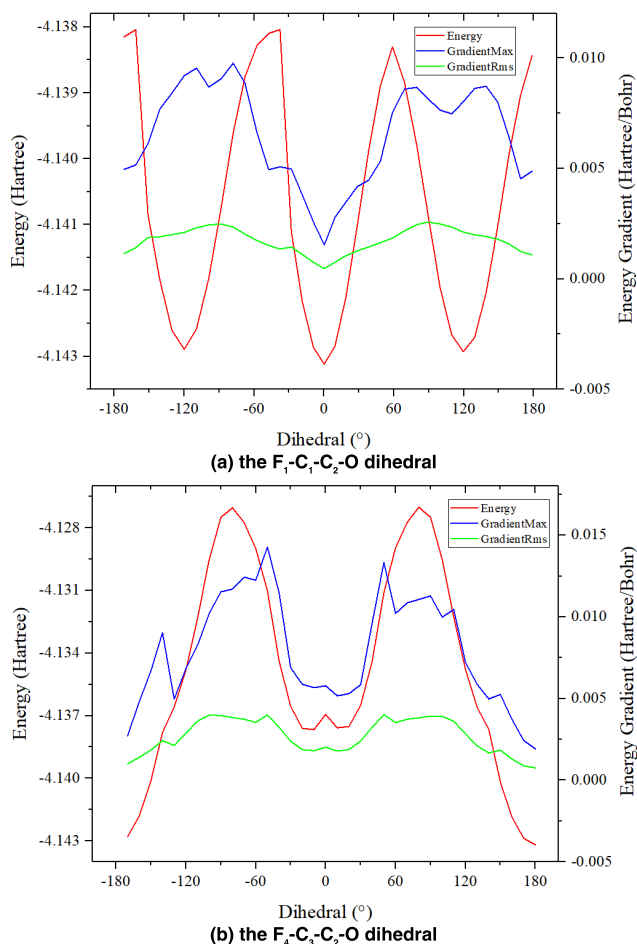

FIGURE 3. (a) and (b) show the rotation of the F_1-C_1-C_2-O dihedral and the F_4-C_3-C_2-O dihedral. The red curve is the molecule energy change during the rotation; the blue curve and the green curve are the energy gradient change's maximum value and root means square value.
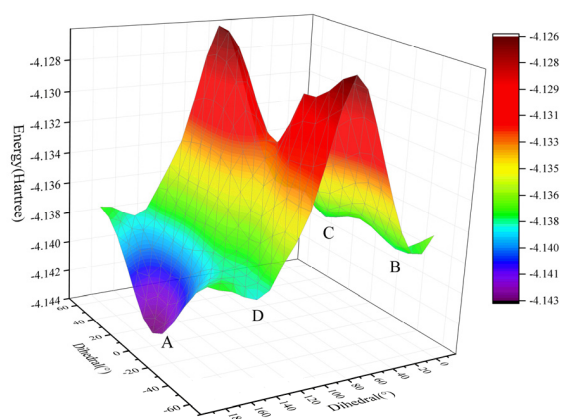

FIGURE 4. Potential energy surface of C5-PFK molecule, the energy in high point is a unstable molecule structure, the energy in low point is a stable molecule structure.

energy of C5-PFK melocule. From the perspective of bond length, C-0 conformer's C_2-C_3 bond is 0.02 Å shorter than the others, while the C_2 =O is only 0.002 Å longer than the others.

TABLE 1. Molecule structure of four C5-PFK conformers.

Conformer		C-0	C-1	C-2	C-3		C-0	C-1	C-2	C-3
Bond Length ($\square$)	C_1-C_2	1.564	1.562	1.563	1.566	C_3-F_4	1.373	1.366	1.366	1.368
	C_2-C_3	1.555	1.575	1.575	1.575	C_4-F_5	1.337	1.336	1.340	1.337
	C_3-C_4	1.559	1.568	1.556	1.561	C_4-F_6	1.338	1.350	1.344	1.348
	C_3-C_5	1.559	1.556	1.569	1.561	C_4-F_7	1.347	1.339	1.341	1.339
	C_1-F_1	1.334	1.344	1.349	1.340	C_5-F_8	1.337	1.344	1.340	1.348
	C_1-F_2	1.346	1.349	1.344	1.343	C_5-F_9	1.339	1.342	1.336	1.339
	C_1-F_3	1.346	1.334	1.334	1.343	C_5-F_{10}	1.348	1.340	1.350	1.338
	C_2-O	1.192	1.190	1.190	1.190					
Bond Dihedral (°)	F_1-C_1-C_2-O	0	-27.9	26.9	60.0	F_5-C_4-C_3-F_4	184.9	-34.8	-60.8	-49.5
	F_4-C_3-C_2-O	179.8	-3.3	3.4	0	F_8-C_5-C_3-F_4	175.1	-58.0	156.0	-69.1
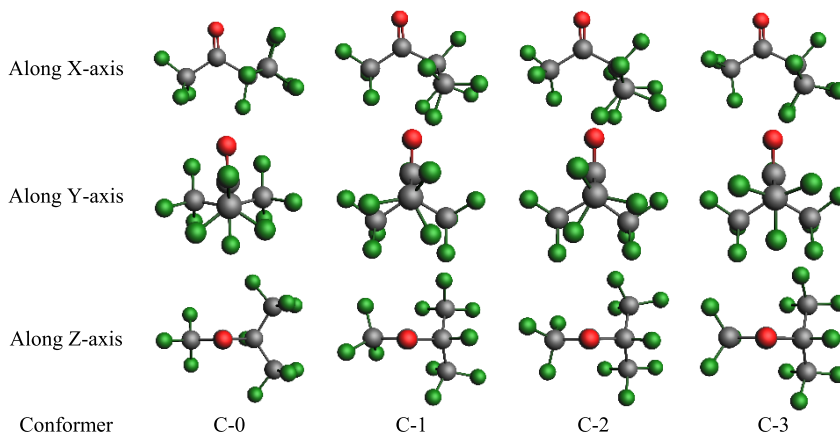
FIGURE 5. View of four conformers of C5-PFK, observed along the X, Y, and Z axes.

TABLE 2. Mayer bond order.

Bond	C-0	C-1	C-2	C-3	Bond	C-0	C-1	C-2	C-3
C_1-C_2	0.9508	0.9617	0.9614	0.9625	C_3-F_4	0.7954	0.8046	0.8045	0.7944
C_2-C_3	0.9183	0.9178	0.9180	0.9163	C_4-F_5	0.8488	0.8359	0.8235	0.8329
C_3-C_4	0.9900	0.9777	0.9832	0.9802	C_4-F_6	0.8312	0.8147	0.8251	0.8208
C_3-C_5	0.9900	0.9833	0.9777	0.9802	C_4-F_7	0.8059	0.8400	0.8288	0.8344
C_1-F_1	0.8447	0.8385	0.8396	0.8359	C_5-F_8	0.8488	0.8252	0.8401	0.8208
C_1-F_2	0.8397	0.8394	0.8386	0.8372	C_5-F_9	0.8312	0.8287	0.8361	0.8344
C_1-F_3	0.8397	0.8402	0.8408	0.8372	C_5-F_{10}	0.8059	0.8234	0.8150	0.8329
C_2=O	1.9327	1.9281	1.9284	1.9190					

From the perspective of bond dihedral, in C-3 conformer, the trifluoromethyl group (CF$_3$·) is rotated by 60° and the heptafluoroisopropyl group (C$_3$F$_7$·) is rotated by 180° compared to C-0 conformer. The C-F bond on the trifluoromethyl group (CF$_3$·) in C-0 conformer appears to be two long and one short, while the C-F bond lengths in C-3 conformer are similar. The C_3-F_4 bond in C-0 conformer's heptafluoroisopropyl group (C$_3$F$_7$·) is about 0.007 Å longer than the others. The two trifluoromethyl groups (CF$_3$·) of heptafluoroisopropyl group (C$_3$F$_7$·) have a similar configuration and are bilateral symmetrical. According to the view along the Y and Z axes, the F_1-C_1-C_2-O dihedrals of the C-1 conformer and C-2 conformer are −27.9° and 26.9°, the F_4-C_3-C_2-O dihedrals are −3.3° and 3.4°, respectively. The trifluoromethyl groups (CF$_3$·) attached to C_4 and C_5 atoms are also similar to each other and approximately mirror symmetrical.

B. FRONTIER MOLECULAR ORBITAL ANALYSIS
1) MAYER BOND ORDER
The bond order is a value in the molecular orbital method that indicates the bonding strength of two adjacent atoms. When a covalent bond is formed, the electrons in the bonding orbital are called bonding electrons, which reduce the energy of the system and help to form a stable bond. In general, the higher the bond order, the more stable the bond. On the contrary, the smaller the bond order, the larger the bond length [36].

The Mayer bond order within the four C5-PFK conformers are listed in Table 2. From an overall perspective, in four conformers, the C_2 = O bond has the highest Mayer bond order; the C-C bond is the secondary, wherein C_2-C_3 is lower than the other C-C bonds; the C-F bond in the trifluoromethyl group (CF$_3$·) comes next; and the C_3-F_4 bond has the lowest Mayer bond order. Because the C_1 and C_3 atoms are directly
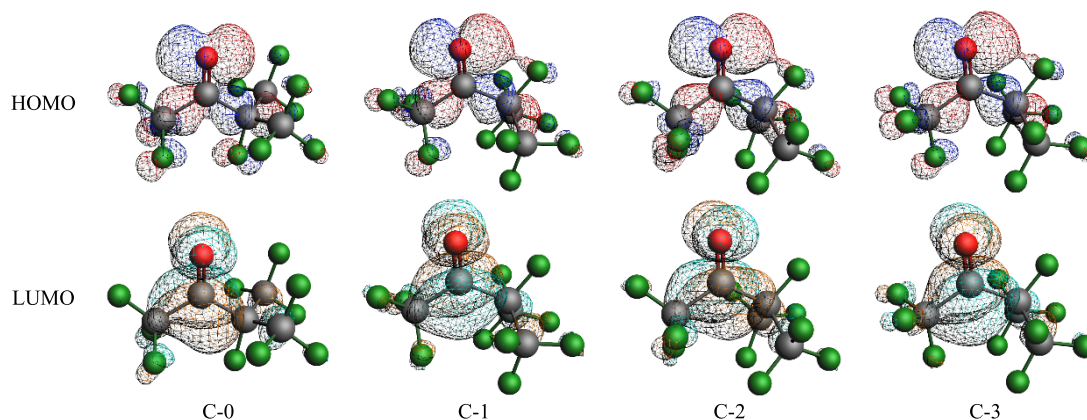
FIGURE 6. HOMO and LUMO wave function of four conformers, red and orange represents positive phase, blue and green represents negative phase.

attached to the carbonyl group (-C = O-), they are weaker than the C-C bonds in heptafluoroisopropyl group ($C_3F_7\cdot$). Due to the effect of trifluoromethyl groups ($CF_3\cdot$) attached to the C_3 atom, which exhibit a more active reactivity, the C_2-C_3 and C_3-F_4 bonds are subjected. So the Mayer bond order of C_2-C_3 bond is the smallest in C-C bonds, and the Mayer bond order of C_3-F_4 bond is much smaller than other C-F bonds.

Since the molecule structure of C-0 conformer is relatively stable, its Mayer bond order of C_1-C_2 bond is about 0.01 lower than the other three; and the C_2-C_3 bond is about 0.0005 higher than C-1 conformer and C-2 conformer, and 0.002 higher than C-3 conformer; its C_3-C_4 bond and C_3-C_5 bond are about 0.01 higher than the other three; C-0 conformer has the highest Mayer bond order of $C_2 = O$ bond, which is 0.004 higher than C-1 conformer and C-2 conformer, and 0.014 higher than C-3. The Mayer bond order of C_3-F_4 bonds in C-0 conformer and C-3 conformer are close, are 0.005 lower than C-1 conformer and C-2 conformer. The Mayer bond order of C_1-C_2, C_2-C_3, $C_2 = O$ bonds are similar in C-1 conformer and C-2 conformer. Since the molecule structure is approximately bilaterally symmetric, the Mayer bond order of C_3-C_4 bond and C_3-C_5 bond, C_1-F_1 bond and C_1-F_2 bond, C-F bonds in the C_4 and C_5 trifluoromethyl groups ($CF_3\cdot$) are approximately equal.

2) MOLECULAR ORBITAL

Frontier molecular orbital theory believes that there are electrons in the molecule similar to the ''valence electrons'' of a single atom. The Highest Occupied Molecular Orbital (HOMO) of a molecule is relatively loose in its electron binding, and has the property of an electron donor. The negative value of the HOMO level represents the ionization energy of the substance. The higher the HOMO level, the lower the ionization energy, indicating that the molecule is more likely to lose electrons. Whereas, the Lowest Unoccupied Molecular Orbital (LUMO) has a stronger affinity for electrons, which shows the property of having an electron acceptor. The lower the LUMO level, indicating that the molecule is more likely to get electrons. These two molecular orbital determine the

electron gain, loss and transfer ability of the molecule, so the frontier molecular orbital and its electrons play a key role in the chemistry reaction between molecules [37].

Fig. 6 shows the phase of the frontier molecular orbital wave function in the four conformers of C5-PFK, indicating the electron distribution state of the frontier molecular. The size of the shadow reflects the probability density of electrons appearing in the area. The larger the shadow, the greater the probability that electrons appear in the area. The HOMO wave function is mainly distributed in the C_1-$C_2 = O$-C_3, C_4-C_3-C_5, F_4 and F atoms in the trifluoromethyl groups ($CF_3\cdot$), in the Y-Z plane. The O atom in the C-1, C-2, C-3 conformers is affected by the F_4 atom on the same side, resulting in an overlap on the HOMO orbital wave function between the C_1-$C_2 = O$-C_3 and the F_4 atom. The LUMO wave function are mainly distributed on the C_1-$C_2 = O$-C_3 and C_4, C_5 atoms in the X-Z plane. Since the C-1 conformer and C-2 conformer are approximately mirror symmetrical. Their wave functions are in opposite phase. Likewise, the wave function phases of C-0 conformer and C-3 conformer are reversed.

The LUMO energy of C-0 conformer and C-3 conformer is around −0.7eV, which is about 0.07eV lower than C-1 conformer and C-2 conformer. The the lower energy indicates that the C-0 conformer and C-3 conformer are easier to gain electron. The HOMO energy of the C-0 conformer is about 0.05eV higher than the other three, and its ionization energy is lower, which makes it easier to lose electrons. The HOMO-LUMO energy gap reflects the ability of electrons to transition from occupied orbital to an empty orbit, so to some extent, it can represent the molecule's ability to participate in chemical reactions [38]. The larger the HOMO-LUMO energy gap value, the less likely the electronic transition is to occur, and the more stable molecule is. It can be seen that the HOMO-LUMO energy gap of C-0 conformer is the largest, C-1, C-2 come next, and C-3 is the smallest. Therefore, the C-3 conformer has a relatively strong ability to participate in the reaction, while C-0 conformer is more stable.
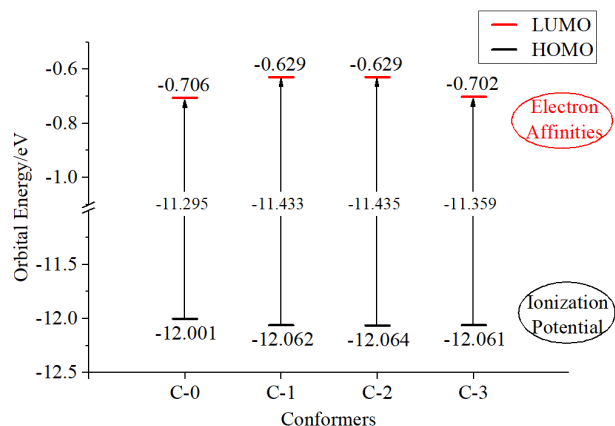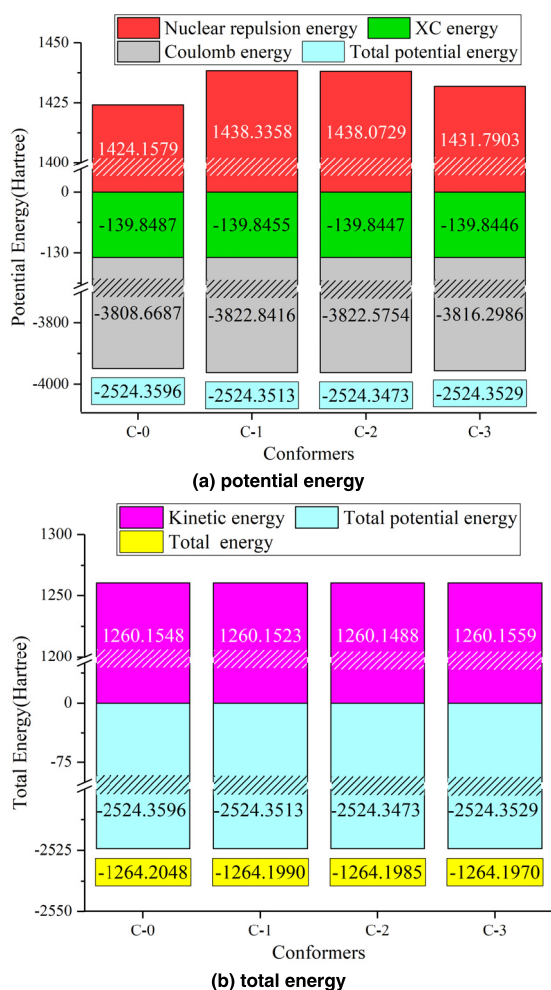
FIGURE 7. Molecular orbital energy level.

(a) potential energy

(b) total energy

FIGURE 8. Energy decomposition diagram of four conformers.

C. ENERGY DECOMPOSITION ANALYSIS

Energy decomposition is an important part of quantum chemical analysis methods. It can decompose the total interaction energy among fragments into physical energy terms to investigate the nature of interactions [39]. In this paper, the total energy of C5-PFK molecule is roughly divided into kinetic energy and potential energy. The kinetic energy includes the internal vibration of molecule. The potential energy includes nuclear repulsion energy, Coulomb energy and exchange-correlation energy.

Compared to other conformers, the C-0 conformer's configuration is more symmetrical, so its nuclear repulsion energy and coulomb energy are the smallest. But C-1 conformer and C-2 conformer has a relatively compact molecule structure, so their nuclear repulsion energy and coulomb energy are the largest. However, the exchange-correlation energy of four conformers is similar. Therefore, when the nuclear repulsion energy and the Coulomb energy are offset, the potential energy difference of four conformers is reduced. The potential energy is sorted from high to low as C-2, C-1, C-3, C-0. The kinetic energy of four conformers is similar, the order from high to low is C-3, C-0, C-1, C-2. The C-0 conformer has a total energy of -1264.2048 Hartree, which is the lowest. The total energy of the C-1 conformer is -1264.1990 Hartree, which is 0.0058 Hartree higher than C-0 conformer; the total energy of the C-2 conformer is -1264.1985 Hartree, which is 0.0063 Hartree higher than C-0; the total energy of the C-3 conformer is -1264.1970 Hartree, which is 0.0078 Hartree higher than C-0. The total energy is ordered from high to low as C-3, C-2, C-1, C-0.

IV. DISCUSSION

In this paper, four possible conformers are obtained by rotating around the single C-C bond attached to the carbonyl group (-C = C-) in the C5-PFK molecule. The C-C bond angle is also variable in C5-PFK molecule. Limited to the computation amount, and due to the structural symmetry of the C5-PFK molecule, all possible conformers are not analyzed and studied in this paper, so the potential energy surface scanning is only part of the most possible conformers.

The Mayer bond of the four conformers can reflect the bond strength of each bond in C5-PFK, which can be used to study the stability and decomposition pathways of C5-PFK insulating gas in the fault state of overheating or discharging in gas-insulated equipment in the future work. The HOMO and LUMO energy in the frontier molecular orbit can reflect its ability to lose and acquire electrons, and the range and phase of wave function will affect the overlap degree of molecular orbital interactions. Then HOMO-LUMO gap can judge the activity of different C5-PFK conformers' participation in the reaction. Through these information, the reaction mechanism of C5-PFK with other carrier gases or impurity gases, and the physical adsorption or chemical reaction on the interface of metals or organic solids can be studied in later studies. The energy decomposition analysis of different conformers can be used for the further study of the difficulty and reaction rate of C5-PFK decomposition reaction.

V. CONCLUSION

In this paper, four possible conformers of C5-PFK molecule were obtained by rotating the F_1-C_1-C_2-O and F_4-C_3-C_2-O dihedrals. These four conformers' molecule

structure are analyzed on the bond length and dihedral for the atomic distribution and symmetry. In the C-0 conformer as the most stable molecule structure, the Mayer bond of C_1-C_2 bond is much smaller than the other three conformers, C_3-F_4 bond is smaller, C_2-C_3 bond is larger, C_3-C_4 and C_3-C_5 bonds are much larger. The Mayer bond order of C-1 conformer and C-2 conformer are mirror symmetrical, which is similar with their molecule structure. The Mayer bond order of C_2-C_3, C_3-F_4, $C_2 = O$ bonds in C-3 conformer are smaller than the other three. According to the frontier molecular orbital analysis, the reactivity from high to low of the four conformers are C-3, C-2, C-1, C-0, wherein the reactivity of C-1 conformer and C-2 conformer are similar. The molecular energy analysis obtained the stability of the four conformers from high to low as C-0, C-1, C-2, C-3.

REFERENCES

[1] X. Zhang, S. Tian, and W. Xiao, "Review of research status of SF$_6$ alternative gas," *Trans. China Electrotech. Soc.*, vol. 33, no. 6, Jun. 2018.

[2] S. L. Reinman, "Intergovernmental panel on climate change (IPCC)," *Encyclopedia Energy Natural Resource Environ. Econ.*, vol. 26, no. 2, pp. 41–42, Feb. 2012.

[3] A. Beroual and A. Haddad, "Recent advances in the quest for a new insulation gas with a low impact on the environment to replace sulfur hexafluoride (SF$_6$) gas in high-voltage power network applications," *Energies*, vol. 10, no. 8, p. 1216, Aug. 2017.

[4] Y. Kieffel, T. Irwin, P. Ponchon, and J. Owens, "Green gas to replace SF$_6$ in electrical grids," *IEEE Power Energy Mag.*, vol. 14, no. 2, pp. 32–39, Apr. 2016.

[5] B. Turner, "United Nations framework convention on climate change," *Rev. Eur. Community Int. Environ. Law*, vol. 1, no. 3, pp. 270–277, Dec. 2010.

[6] A. Mota-Babiloni, J. Navarro-Esbrí, Á. Barragán-Cervera, F. Molés, and B. Peris, "Analysis based on EU Regulation No 517/2014 of new HFC/HFO mixtures as alternatives of high GWP refrigerants in refrigeration and HVAC systems," *Int. J. Refrig.*, vol. 52, pp. 21–31, Apr. 2015.

[7] H. Zhao, *Study on Insulation Performance of C$_4$F$_8$ and CF$_4$ Mixed Gases*. Shanghai, China: SJTU, 2006.

[8] J.-M. Biasse, E. Otegui, and B. T.-V. Keiser, "Benefits of proper SF$_6$ handling to reduce SF$_6$ emissions for sustainable electricity transmission and distribution," in *Proc. CICED*. Sep. 2010, pp. 1–6.

[9] M. Rabie and C. M. Franck, "Assessment of ECO-friendly gases for electrical insulation to replace the most potent industrial greenhouse gas SF$_6$," *Environ. Sci. Technol.*, vol. 52, no. 2, pp. 369–380, Dec. 2017.

[10] X. Li, H. Zhao, and A. B. Murphy, "SF$_6$-alternative gases for application in gas-insulated switchgear," *J. Phys. D, Appl. Phys.*, vol. 51, no. 15, Mar. 2018, Art. no. 153001.

[11] P. Simka and N. Ranjan, "Dielectric strength of C5 perfluoroketone," in *Proc. IS*, Pilsen, Czech Republic, Aug. 2015, pp. 23–28.

[12] M. Hyrenbach and S. Zache, "Alternative insulation gas for medium-voltage switchgear," in *Proc. IEEE PCIC Europe*, Berlin, Germany, Jun. 2016, pp. 1–9.

[13] E. K. Watkins and W. L. Jorgensen, "Perfluoroalkanes: Conformational analysis and liquid-state properties from *ab initio* and Monte Carlo calculations," *J. Phys. Chem. A*, vol. 105, no. 16, pp. 4118–4125, Mar. 2001.

[14] J. R. Durig, S. W. Hur, T. K. Gounev, F. Feng, and G. A. Guirgis, "Conformational analysis, barriers to internal rotation, vibrational assignment, and ab Initio calculations of 3-fluoro-1-butene," *J. Phys. Chem. A*, vol. 105, no. 17, pp. 4216–4225, Apr. 2001.

[15] T. W. Bates and W. H. Stockmayer, "Conformational energies of perfluoroalkanes. III. Properties of polytetrafluoroethylene," *Macromolecules*, vol. 1, no. 1, pp. 17–24, Jun. 1968.

[16] O. Borodin, G. D. Smith, and D. Bedrov, "A quantum chemistry based force field for perfluoroalkanes and poly(tetrafluoroethylene)," *J. Phys. Chem. B*, vol. 106, no. 38, pp. 9912–9922, Sep. 2016.

[17] S. Tsuzuki, T. Uchimaru, and K. Tanabe, "Conformational analysis of n-alkanes using density functional theory. Comparison with *ab initio* calculations," *Chem. Phys. Lett.*, vol. 246, nos. 1–2, pp. 9–12, Nov. 1995.

[18] J. R. Durig, H. V. Phan, T. S. Little, and B. J. Van Der Veken, "Conformational analysis and structural determinations from *ab initio* calculations for chloroacetaldehyde," *J. Mol. Struct., Theochem*, vol. 202, pp. 143–157, Dec. 1989.

[19] S. Tsuzuki, T. Uchimaru, M. Mikami, and S. Urata, "Magnitude and orientation dependence of intermolecular interaction between perfluoroalkanes: High level *ab initio* calculations of CF$_4$ and C$_2$F$_6$ dimers," *J. Chem. Phys.* vol. 116, no. 8, pp. 3309–3315, Feb. 2002.

[20] X. Zhang, Y. Li, S. Tian, S. Xiao, D. Chen, J. Tang, and R. Zhuo, "Decomposition mechanism of the C5-PFK/CO$_2$ gas mixture as an alternative gas for SF$_6$," *Chem. Eng. J.*, vol. 336, pp. 36–48, Mar. 2017.

[21] P. Deslongchamps, C. Lebreux, and R. Taillefer, "The importance of conformation of the tetrahedral intermediate in the hydrolysis of amides. selective cleavage of the tetrahedral intermediate controlled by orbital orientation," *Can. J. Chem.*, vol. 51, no. 10, pp. 1665–1669, Feb. 2011.

[22] M. Cecchini, "Quantum corrections to the free energy difference between peptides and proteins conformers," *J. Chem. Theory Comput.*, vol. 11, no. 9, pp. 4011–4022, Jul. 2015.

[23] Y. Li, X. Zhang, S. Xiao, D. Chen, Q. Chen, and D. Wang, "Theoretical evaluation of the interaction between C5-PFK molecule and Cu (1 1 1)," *J. Fluorine Chem.*, vol. 208, pp. 48–54, Apr. 2018.

[24] H. Kang, J. Noh, E.-O. Ganbold, D. Uuriintuya, M. S. Gong, J. J. Oh, and S.-W. Joo, "Adsorption changes of cyclohexyl isothiocyanate on gold surfaces," *J. Colloid Interface Sci.*, vol. 336, no. 2, pp. 648–653, Aug. 2009.

[25] R. Cortese, D. Duca, and V. A. S. Herrera, "L-arabinose conformers adsorption on ruthenium surfaces: A DFT study," *J. Phys. Chem. C*, vol. 116, no. 28, pp. 14908–14916, Jun. 2012.

[26] G. te Velde, F. M. Bickelhaupt, E. J. Baerends, C. F. Guerra, S. J. A. van Gisbergen, J. G. Snijders, and T. Ziegler, "Chemistry with ADF," *J. Comput. Chem.*, vol. 22, no. 9, pp. 931–967, Jul. 2001.

[27] C. F. Guerra, J. G. Snijders, G. te Velde, and E. J. Baerends, "Towards an order-N DFT method," *Theor. Chem. Accounts*, vol. 99, no. 6, pp. 391–403, Nov. 1998.

[28] E. J. Baerends, T. Ziegler, and J. Autschbach, "ADF2019, SCM, theoretical chemistry," Vrije Univ., Amsterdam, The Netherlands. [Online]. Available: http://www.scm.com

[29] J. Tiradorives and W. L. Jorgensen, "Performance of B3LYP density functional methods for a large set of organic molecules," *J. Chem. Theory Comput.*, vol. 4, no. 2, pp. 297–306, Jan. 2008.

[30] J. Li, "An *ab initio* study of intermolecular interaction of hydrogen fluoride tetramer," *J. Theor. Comput. Chem.*, vol. 5, no. 2, pp. 187–196, 2006.

[31] N. B. de Lima, V. H. Rusu, and M. N. Ramos, "Hydrogen bonds between phthalimide and hydrogen fluoride: A theoretical study," *Int. J. Quantum Chem.*, vol. 111, nos. 7–8, pp. 1387–1394, Jun./Jul. 2011.

[32] X. Li, X. Guo, A. B. Murphy, H. Zhao, J. Wu, and Z. Guo, "Calculation of thermodynamic properties and transport coefficients of C$_5$F$_{10}$O-CO$_2$ thermal plasmas," *J. Appl. Phys.*, vol. 122, no. 14, Oct. 2017, Art. no. 143302.

[33] X. Zhang, Y. Li, S. Xiao, J. Tang, S. Tian, and Z. Deng, "Decomposition mechanism of C$_5$F$_{10}$O: An environmentally friendly insulation medium," *Environ. Sci. Technol.*, vol. 51, no. 17, pp. 10127–10136, Jul. 2017.

[34] L. Goerigk, "How do DFT-DCP, DFT-NL, and DFT-D3 compare for the description of london-dispersion effects in conformers and general thermochemistry," *J. Chem. Theory Comput.*, vol. 10, no. 3, pp. 968–980, Jan. 2014.

[35] J. Tao, J. P. Perdew, and A. Ruzsinszky, "Long-range Van der Waals interaction," *Int. J. Mod. Phys. B*, vol. 27, no. 18, 2013, Art. no. 1330011.

[36] A. J. Bridgeman, G. Cavigliasso, and L. R. Ireland, "The Mayer bond order as a tool in inorganic chemistry," *J. Chem. Soc. Dalton Trans.*, vol. 14, pp. 2095–2108, Jul. 2001.

[37] D. Tang and P. Yang, "Front line molecular orbital and chemical reactivity," *J. Shanxi Univ., Natural Sci. Ed.*, vol. 1, pp. 26–46, 1978.

[38] J. Aihara, "Reduced HOMO-LUMO gap as an index of kinetic stability for polycyclic aromatic hydrocarbons," *J. Phys. Chem. A*, vol. 103, no. 37, pp. 7487–7495, Aug. 1999.

[39] M. von Hopffgarten and G. Frenking, "Energy decomposition analysis," *Wiley Interdiscipl. Rev. Comput. Mol. Sci.*, vol. 2, no. 1, pp. 43–62, Jan./Feb. 2015.
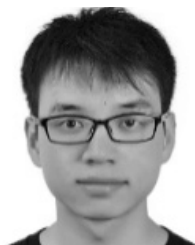
ZHICHENG LEI was born in Fuding, Hubei Province, China, in 1994. He received the bachelor's degree in electrical engineering from Chongqing University, Chongqing, China. He is currently pursuing the master's degree with Wuhan University, China. His research interests include environmentally friendly insulating gas, GIS condition monitoring, and fault diagnosis.

FUPING ZENG was born in Chongqing, China, in 1984. He received the bachelor's degree in electrical engineering from Dalian Maritime University, the master's and Ph.D. degrees from Chongqing University, and the Postdoctoral degree from Wuhan University. He is currently a Professor with Wuhan University, China. His research interests include online monitoring and fault diagnosis of HV electric equipment insulation.

JU TANG was born in Pengxi, Sichuan Province, China, in 1960. He received the bachelor's degree from Xi'an Jiaotong University, and the master's and Ph.D. degrees from Chongqing University. He is a Professor with Wuhan University, a Professor with the State Key Laboratory of Power Transmission Equipment and System Security and New Technology, Chongqing University, China, and the Chief Scientist presiding over the National Basic Research Program of China (973 Program) (2009CB724500). His research interests include online monitoring and fault diagnosis of HV electric equipment insulation.

ZHAOFENG WAN was born in 1995. He received the bachelor's degree in electrical engineering from Chongqing University, Chongqing, China. He is currently pursuing the master's degree with Wuhan University, China.

MINGXUAN ZHANG was born in 1995. She received the bachelor's degree in electrical engineering from Chongqing University, Chongqing, China. She is currently pursuing the master's degree with Wuhan University, China.

LIANGJUN DAI was born in 1996. She received the bachelor's degree in electrical engineering from Chongqing University, Chongqing, China. She is currently pursuing the master's degree with Wuhan University, China.

• • •