Theoretical calculation of total electron-impact ionization cross section of $\text{C}_6\text{F}_{12}\text{O}$

Cite as: AIP Advances 10, 035217 (2020); https://doi.org/10.1063/1.5133830
Submitted: 30 October 2019. Accepted: 01 March 2020. Published Online: 17 March 2020

Yang Wang, Shuangshuang Tian, Xiaoxing Zhang, Wei Liu, Yufei Wang, and Guozhi Zhang

© 2020 Author(s).
Theoretical calculation of total electron-impact ionization cross section of \( \text{C}_6\text{F}_{12}\text{O} \)

Yang Wang,1 Shuangshuang Tian,2,a) Xiaoxing Zhang,2 Wei Liu,3 Yufei Wang,2 and Guozhi Zhang2

AFFILIATIONS
1 Wuhan Electric Power Technical College, Wuhan 430079, China
2 Key Laboratory for High-Efficiency Utilization of Solar Energy and Operation Control of Energy Storage System, Hubei University of Technology, Wuhan 430068, China
3 Electric Power Research Institute of State Grid Anhui Electric Power Co., Ltd, Hefei 230000, China

a) Author to whom correspondence should be addressed: tianshuang1002@yahoo.com

ABSTRACT
\( \text{C}_6\text{F}_{12}\text{O} \) can be used in gas-insulated equipment due to its excellent insulation properties. The purpose of this paper is to calculate the total electron-impact ionization cross section to evaluate the dielectric strength of the molecule using the Deutsch–Märk formula. First, according to the calculation method of quantum chemistry, the structure of the molecule is optimized. Three different methods, such as Mulliken population analysis, C-squared population analysis, and natural atomic orbital (NAO), are used to calculate the molecular orbital components, and then the molecular collision cross section is obtained. The influence of different weighting factors on the calculation results is analyzed. The validity of the proposed method is verified by the calculation results of \( \text{H}_2\text{O}, \) \( \text{C}_3\text{H}_6\text{O}, \) and \( \text{C}_5\text{F}_{10}\text{O}. \) The results show that the calculation value with the NAO method is closer to the experimental results, which provides a reference for the calculation and analysis of the collision cross section of \( \text{C}_6\text{F}_{12}\text{O}. \) The calculation results in this paper can provide basic data for further calculation of the dielectric strength of \( \text{C}_6\text{F}_{12}\text{O}. \)

© 2020 Author(s). All article content, except where otherwise noted, is licensed under a Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by/4.0/). https://doi.org/10.1063/1.5133830

I. INTRODUCTION

\( \text{SF}_6 \) is widely used in electrical equipment such as gas insulated switchgear (GIS), gas insulated transmission line (GIL), gas insulation transformers (GIT), and other gas insulated equipment. However, due to the extremely high potential value of the greenhouse effect and the toxicity of the decomposition products,1,2 the call for limiting its use is getting higher. The search for a safe and environmentally friendly new insulating gas medium has become an urgent requirement for the sustainable development of the power industry.3,4

\( \text{C}_6\text{F}_{12}\text{O} \) is a non-flammable material that is harmless to the environment. It was originally used as a fire extinguishing agent to replace the halon series to reduce the damage to the ozone layer.5 In recent years, the research on \( \text{SF}_6 \) alternative gas has made us pay attention to it. The insulation performance of \( \text{C}_6\text{F}_{12}\text{O} \) is about 2.7 times that of \( \text{SF}_6. \) Under the influence of liquefaction temperature, the medium needs to be used with buffer gas, and the mixing ratio is generally controlled below 6%. Adding 3% \( \text{C}_6\text{F}_{12}\text{O} \) to \( \text{N}_2 \) can increase the power frequency breakdown voltage by 90%. The breakdown products and thermal decompositions are mainly fluorocarbons, such as \( \text{CF}_4, \) \( \text{C}_2\text{F}_6, \) and \( \text{C}_3\text{F}_8. \) These gases are all alternative gases with better insulation properties and have a smaller impact on the environment than \( \text{SF}_6. \)5–10 These studies have initially shown that \( \text{C}_6\text{F}_{12}\text{O} \) mixtures have the potential to be used as gas insulating media in electrical equipment, especially in medium and low voltage equipment.

Yu et al. used quantum chemistry to verify that \( \text{C}_6\text{F}_{12}\text{O} \) has a large surface area, which is one of the factors that influences its high insulation performance, but there is no collision cross section data for reference.11 In order to research the insulation performance and the physical behavior of the gas discharge process in a more in-depth theoretical study, the study of the collision cross section helps to study the hindrance of gas to electron motion during discharge and calculate the relevant electron swarm parameters, such as the ionization coefficient and critical breakdown field. The accuracy and
validity of the Deutsch–Märk (DM) formula have been verified in the calculation of atoms, molecules, ions, and various free radicals.\textsuperscript{12} The DM formula is used to calculate the ionization cross section and the attachment cross section. Xiong \textit{et al.} calculated the electron-impact cross sections of two alternative gases of SF\textsubscript{6}, C\textsubscript{2}H\textsubscript{4}O, and C\textsubscript{2}F\textsubscript{2}N, and discussed the influence of different basis sets on the calculation results. At the same time, the weight coefficient is corrected so that the calculated value agrees with the measured value.\textsuperscript{11} In addition, the Binary-Encounter-Dipole (BED) model for calculating electron-impact ionization cross sections for atoms and molecules is presented, which combines the binary-encounter theory with the dipole interaction of the Bethe theory for fast incident electrons.\textsuperscript{14,15} The Binary-Encounter-Bethe (BEB) model is a simpler version of the BED approach.\textsuperscript{16} In the literature,\textsuperscript{17–20} the collision cross section of C\textsubscript{2}H\textsubscript{3}O (x = 1–5) gas was calculated by DM and BEB. It was found that the DM method is closer to the measured value. Since there are many atoms involved in the molecule, there is no precedent for the calculation of the attachment dissociation process. Therefore, the electron impact ionization is calculated according to the DM formula in this paper. For the composition calculation of molecular orbitals in the references, the method of Mulliken population analysis (MPA) is used to calculate the basis function and the addition method is used to calculate the contribution of the atomic orbit to the molecular orbital.\textsuperscript{19,20} This method lacks physical meaning in the processing of the cross term of the basis functions, which may cause inaccurate calculation,\textsuperscript{21} so this paper will use C-squared population analysis (SCPA) and natural atomic orbital (NAO) to directly calculate the contribution of the atomic orbit and make the comparison with MPA.

First, the calculation method of DM is summarized, and the methods of MPA, SCPA, and NAO are compared. Different methods were used for calculating the electron-impact cross section of H\textsubscript{2}O, C\textsubscript{2}H\textsubscript{4}O, and C\textsubscript{2}F\textsubscript{2}O, which are compared with the experimental values to analyze the accuracy of different methods. At the same time, the influence of different weight factors on the results is analyzed. Finally, the electron impact ionization cross sections of C\textsubscript{2}F\textsubscript{2}O were calculated by these methods, and the results are given in this paper. The calculations in this paper provide a basis for in-depth calculation of parameters, such as ionization coefficient and critical breakdown field during gas discharge.

II. THEORETICAL METHOD

A. DM formula

The Deutsch–Märk formula was, which been described in the literature.\textsuperscript{19–21} the method that can be used to calculate the electron-impact ionization cross section of atomic, molecules, ions, and clusters.

DM formula calculation of the total cross section of molecules has the form

\[
\sigma = \sum_j g_j \rho(r_j)^2 f(U),
\]

with

\[
f(U) = d(1/U)[(U - 1)/(U + 1)]^a \\
\times b[ b + c[ 1 - 1/2U ] \ln[ 2.7 + (U - 1)^{0.5} ]],
\]

where \( j \) represents the molecular orbital number, \( g_j \) is the weighting factor, \( r_j \) is the radius of maximum radial density of the subshells,\textsuperscript{21} and \( U \) is the reduced energy, which is equal to \( E/E_j \), where \( E \) is the energy of incident electron and \( E_j \) is the ionization energy of the \( j \)th subshell. The parameters \( a, b, c, \) and \( d \) in the function \( f(U) \) are listed in Ref. \textsuperscript{12}, \( a = 3/2, b = 1, c = 2/3, \) and \( d = 1 \). Based on Ref. \textsuperscript{13}, the \( g_j, f(U) \), and \( j \) are obtained from the population analysis. There are different methods to calculate the population in this paper.

B. The population analysis of molecular orbitals

Calculating the orbital component means the contribution of the various components that make up the orbit. The parameters involved in the DM are the contributions of atomic orbitals. We used different methods to calculate the population in this paper. No one method is absolutely correct. The orbital component is not observable, and the definition is completely artificial. In this paper, two methods are used to calculate the atomic orbital distribution—the additive basis function contribution method and the NAO method. The calculation method of the basis function is divided into the MPA method and SCPA method.

The wave function of the orbit is a linear form of the basis function. In general, there are cross terms for the contribution of different basis functions to the orbit. In fact, there are two different ways of dealing with cross terms—MPA and SCPA. The difference between the two is that MPA distributes the intersections between the basis functions evenly.\textsuperscript{21–24} In SCPA, the orbital components are calculated by the square of the coefficients and normalized.\textsuperscript{25,26} In MPA, the result of the calculation sometimes has a meaningless negative component value. Both methods can obtain the contribution of the basis function to the molecular orbital, and then, the contribution of the atomic orbital to the molecular orbital is obtained by the addition method.

In addition, methods for calculating atomic orbital contributions can be analyzed by means of natural bond orbital (NBO).\textsuperscript{27,28} The NBO analysis can be obtained from the density matrix information of the system (NAO), and the number of NAOs is the same as the basis function. Since NAOs are orthogonal to each other, it is not necessary to consider how to divide the cross terms, so the square of the coefficient of NAO in the corresponding orbit is its composition in the orbit. The stability of the NAO method is significantly better than that of the additive basis function, which can converge quickly as the quality of the base group increases, and the principles are strict.\textsuperscript{29–33}

In theory, when calculating the atomic orbital contribution of molecular orbitals, SCPA is more reasonable for calculating the contribution of the basis function, and the NAO method is more accurate for calculating the contribution of atomic orbitals. In this paper, the calculation of H\textsubscript{2}O, C\textsubscript{2}H\textsubscript{4}O, and C\textsubscript{2}F\textsubscript{2}O is used to verify the validity of the calculation method, and the C\textsubscript{2}F\textsubscript{2}O are calculated and compared.

III. CALCULATION PROCESS AND RESULT ANALYSIS

In this paper, Gaussion09 is used to calculate the orbital parameters of the molecule, and the orbit is analyzed by Multiwfn.\textsuperscript{25} Since the molecular structure involved is similar to C\textsubscript{2}F\textsubscript{2}O, we choose the same basis set as in Ref. \textsuperscript{13} for calculation, that is, using...
There are two kinds of weight factors, which are from Refs. 12 and 13, as shown in Table I. The influence of different weight factors is also discussed in this paper. The values of the weighting factors in the calculation are shown in Table I.

### A. Method validation

The molecules of H$_2$O, C$_3$H$_6$O, and C$_5$F$_{12}$O are calculated using the methods described in this paper, and the calculated results are compared with the reference data.

#### 1. H$_2$O

Table II shows the calculation results of all the orbitals of the H$_2$O molecule. There are five molecular orbitals in which the valence electrons occupy four orbitals. The orbital 1 is the inner orbit of the molecule, and it does not participate in the bonding.

The calculation results of the electron collision cross section of H$_2$O are shown in Fig. 1, wherein the weight coefficient is from Refs. 12 and 13. Comparing the three calculation methods with the measured values, it is found that the cross sections obtained by the three calculation methods are consistent with the change trend of electron energy, and the peak value is obtained at about 100 eV. The peak value of MPA is about 2.43 Å$^2$, and the peak value of SCPA is the lowest with 1.97 Å$^2$. Before the peak is reached, the results of SCPA are in good agreement with the measurements, and after the peak, it seems that MPA and NAO are closer to the measured values. The measured values are derived from the literature.

It can be seen from Fig. 1 that after the correction, the cross sections obtained by the three methods are reduced compared with the weighting factor from Ref. 13, and the results of NAO are closer to the experimental measurements.

#### 2. C$_3$H$_6$O

The molecules of C$_3$H$_6$O have a total of 16 molecular orbitals, and the valence electrons participating in the cross section calculation occupy 12 orbitals. Table III shows the parameters of all valence electrons occupying the orbit, consistent with the results in Ref. 13.

The calculation of the collision section is shown in Fig. 2, where the measured value is derived from Ref. 33. Similar to the calculation results of H$_2$O, the calculated value is slightly larger than the experimental value, and the data calculated by the SCPA method are closest to the measured value. Using the modified weight coefficients, the data obtained by the NAO method are closer to the measured value.

#### 3. C$_5$F$_{12}$O

There are 64 molecular orbitals in C$_5$F$_{12}$O of which 48 are involved in the calculation. Table IV shows the parameter values of the five highest occupied orbitals. The energy values in Table IV and the parameter values of the MPA calculation method are consistent with the calculation results in the literature. The molecular collision cross section of C$_5$F$_{12}$O is calculated, as shown in Fig. 3. The reference data are from the literature. It can be seen that the calculation results of NAO are in good agreement with the results of the literature. The calculated value of MPA is slightly larger than that of NAO, and SCPA has a significantly higher.

### Table I. The weighting factor of HCF$_O$.

| Electron number in subshell | E$_j$×g$_j$ | O | F | C |
|----------------------------|------------|---|---|---|
| 1S,1                       | 38.2       | ... | ... | ... |
| 1S,2                       | 70         | ... | ... | ... |
| 2S,1                       | 12         | 15.12 | 14.40 | 15.00 |
| 2S,2                       | 20         | 25.20 | 24.00 | 25.00 |
| 2P,1                       | 32.5       | 24.38 | 24.70 | 26.00 |
| 2P,2                       | 30         | 22.50 | 22.80 | 24.00 |

B3LYP/6-311G** for structural optimization and HF/6-311G** for orbital analysis.

FIG. 1. The cross section of H$_2$O (weighting factor in Refs. 12 and 13).

### Table II. Molecular orbital distribution of H$_2$O.

| MO | E$_j$ | Atomic orbital | ξ$_j$ | Mulliken | SCPA | NAO |
|----|------|----------------|-------|----------|------|-----|
| 5  | 12.6 | O 2p           | 2     | 2        | 2    |
| 4  | 14.7 | H 1s           | 0.176 | 0.160    | 0.121|
|    |      | O 2s           | 0.264 | 0        | 0.242|
|    |      | O 2p           | 1.560 | 1.840    | 1.637|
| 3  | 18.5 | H 1s           | 0.767 | 0.176    | 0.569|
|    |      | O 2s           | 0     | 0.533    | 0    |
|    |      | O 2p           | 1.233 | 1.291    | 1.431|
| 2  | 32.2 | H 1s           | 0.338 | 0.090    | 0.397|
|    |      | O 2s           | 1.565 | 1.842    | 1.509|
|    |      | O 2p           | 0.097 | 0.068    | 0.094|
| 1  | 539.7| O 1s           | 2     | 2        | 2    |
TABLE III. Molecular orbital distribution of C$_3$H$_6$O.

| MO j | $E_j$ (eV) | Atomic orbital | Mulliken | SCPA | NAO |
|------|------------|----------------|----------|------|-----|
| 16   | 11.453     | H 1s           | 0.021    | 0.0416 | 0.0504 |
|      |            | C 2s           | 0.0237   | 0.6864 | 0.0206 |
|      |            | C 2p           | 0.5148   | 0.6586 | 0.6374 |
|      |            | O 2p           | 1.440    | 0.6134 | 1.2916 |
| 15   | 13.041     | H 1s           | 0.2998   | 0.1742 | 0.1912 |
|      |            | C 2s           | 0        | 0.0352 | 0    |
|      |            | C 2p           | 0.5656   | 0.6216 | 0.5512 |
|      |            | O 2p           | 1.1346   | 1.169  | 1.2576 |
| 14   | 14.715     | H 1s           | 0.7568   | 0.5898 | 0.6836 |
|      |            | C 2s           | 0        | 0.2532 | 0    |
|      |            | C 2p           | 1.1742   | 1.03   | 1.185 |
|      |            | O 2p           | 0.069    | 0.127  | 0.1314 |
| 13   | 15.218     | H 1s           | 0.4236   | 0.3812 | 0.4166 |
|      |            | C 2s           | 0        | 0.0512 | 0    |
|      |            | C 2p           | 0.76     | 0.8896 | 0.9332 |
|      |            | O 2s           | 0.1354   | 0.102  | 0.055 |
|      |            | O 2p           | 0.681    | 0.576  | 0.5952 |
| 12   | 15.381     | H 1s           | 0.8982   | 0.7634 | 0.779 |
|      |            | C 2s           | 0        | 0.1766 | 0    |
|      |            | C 2p           | 1.11072  | 1.06   | 1.221 |
| 11   | 17.070     | H 1s           | 0.4848   | 0.65   | 0.544 |
|      |            | C 2p           | 0.984    | 1.17   | 1.3052 |
|      |            | O 2s           | 0.19     | 0      | 0    |
|      |            | O 2p           | 0.3412   | 0.18   | 0.1508 |
| 10   | 17.298     | H 1s           | 0.6028   | 0.3236 | 0.3986 |
|      |            | C 2s           | 0        | 0.0576 | 0    |
|      |            | C 2p           | 1.2332   | 0.8772 | 1.068 |
|      |            | O 2s           | 0        | 0.4044 | 0.1286 |
|      |            | O 2p           | 0.164    | 0.3372 | 0.466 |
| 9    | 17.721     | H 1s           | 0.3938   | 0.1238 | 0.3  |
|      |            | C 2s           | 0        | 0.8112 | 0    |
|      |            | C 2p           | 1.3108   | 0.7944 | 1.2028 |
|      |            | O 2p           | 0.2954   | 0.2706 | 0.4972 |
| 8    | 20.322     | H 1s           | 0.4014   | 0.1204 | 0.3402 |
|      |            | C 2s           | 0.6534   | 1.179  | 0.4514 |
|      |            | C 2p           | 0.6464   | 0.2228 | 0.6548 |
|      |            | O 2s           | 0.1618   | 0.3458 | 0.2032 |
|      |            | O 2p           | 0.137    | 0.132  | 0.3504 |
| 7    | 26.599     | H 1s           | 0.4796   | 0.1626 | 0.597 |
|      |            | C 2s           | 1.328    | 1.7564 | 1.064 |
|      |            | C 2p           | 0.1924   | 0.081  | 0.3246 |
|      |            | O 2p           | 0        | 0      | 0.0144 |

(Continued.)

TABLE III. (Continued.)

| MO j | $E_j$ (eV) | Atomic orbital | Mulliken | SCPA | NAO |
|------|------------|----------------|----------|------|-----|
| 6    | 28.619     | H 1s           | 0.3242   | 0.1014 | 0.4248 |
|      |            | C 2s           | 1.3786   | 1.627  | 1.1774 |
|      |            | C 2p           | 0.1758   | 0.0562 | 0.2758 |
|      |            | O 2s           | 0.1214   | 0.2154 | 0.114 |
|      |            | O 2p           | 0        | 0      | 0.008 |
| 5    | 37.928     | H 1s           | 0        | 0.0072 | 0.0072 |
|      |            | C 2s           | 0.3496   | 0.347  | 0.3808 |
|      |            | C 2p           | 0.1316   | 0.0548 | 0.251 |
|      |            | O 2s           | 1.3484   | 1.5358 | 1.2298 |
|      |            | O 2p           | 0.1704   | 0.0552 | 0.1312 |

value than the reference. This method may not be applicable to the calculation of macromolecules. The calculated values with the modified weight factor show a small decrease, and the NAO method drops by about 10% at the highest value. The result of the BEB model is also shown in Fig. 3, which is similar to MPA$^{12}$ calculation results.

B. Calculation and analysis of C$_6$F$_{12}$O

The molecules of C$_6$F$_{12}$O have a total of 323 molecular orbitals of which 76 electrons occupy the orbit. The typical orbital distribution is shown in Fig. 4: (a) the lowest unoccupied molecular orbital, (b) the highest occupied molecular orbital, (c) the lowest valence electron occupied orbit, and (d) the highest molecular inner orbit.

In the 76 electron-occupying orbitals, the valence electrons participating in the cross section calculation occupy 57 orbitals (the number of molecular orbitals is 20–76). Table V shows the parameter values for the five highest occupied orbits.

FIG. 2. Molecular cross section of C$_3$H$_6$O (weighting factor in Refs. 12 and 13).
TABLE IV. Five highest electron occupation orbit distribution parameters of $C_5F_{10}O$.

| MO | $E_j$ | Atomic orbital | Mulliken | SCPA   | NAO   |
|----|-------|----------------|----------|--------|-------|
| 64 | 13.970| $C$ 2s         | 0.0698   | 1.3141| 0.0500|
|    |       | $C$ 2p         | 0.6357   | 0.3827| 0.4812|
|    |       | $O$ 2p         | 1.0660   | 0.1680| 1.1460|
|    |       | $F$ 2p         | 0.2285   | 0.1075| 0.3228|
| 63 | 15.843| $C$ 2s         | 0.0712   | 0.8157| 0.0366|
|    |       | $C$ 2p         | 0.7983   | 0.5072| 0.6998|
|    |       | $O$ 2p         | 0.4776   | 0.3658| 0.8724|
|    |       | $F$ 2p         | 0.6529   | 0.3113| 0.3912|
| 62 | 17.061| $C$ 2s         | 0.0162   | 1.3763| 0.0274|
|    |       | $C$ 2p         | 0.6972   | 0.3233| 0.6610|
|    |       | $O$ 2p         | 0.7310   | 0.0542| 0.3560|
|    |       | $F$ 2p         | 0.5556   | 0.2462| 0.9555|
| 61 | 17.704| $C$ 2s         | 0.1026   | 1.5295| 0.1244|
|    |       | $C$ 2p         | 0.5602   | 0.2462| 0.3798|
|    |       | $O$ 2p         | 0.2802   | 0.0434| 0.3980|
|    |       | $F$ 2p         | 1.0424   | 0.1808| 1.0978|
| 60 | 18.414| $C$ 2s         | 0.0404   | 0.9092| 0.0475|
|    |       | $C$ 2p         | 0.4366   | 0.3010| 0.3564|
|    |       | $O$ 2s         | 0.0206   | 0.0417| 0.0555|
|    |       | $O$ 2p         | 0.4318   | 0.1858| 0.5008|
|    |       | $F$ 2s         | 1.0706   | 0.5623| 1.0398|

Figure 5 shows the calculation results of the electron impact ionization cross section of $C_5F_{10}O$. The difference between the two weight coefficients obtained by the same calculation method is not significant. Under MPA and NAO, the weighting factor using the literature is slightly smaller. The result of the BEB is similar to MPA result.

It can be seen that the cross section values calculated by SCPA are significantly larger than the other two methods. In the literature, the maximum value of $C_6F_{12}O$ cross section data is about 15 Å$^2$. The molecule of $C_6F_{12}O$ has a similar molecular...
structure and the number of atoms is large, so the maximum value should be slightly larger than 15 Å. Comparing the calculation results, it seems more reasonable to use the MPA and NAO methods.

| MO j | Ej | Atomic orbital | ξj | Mulliken | SCPA | NAO |
|------|----|----------------|----|----------|------|------|
| 76   | 15.070 | C 2s | 0.083 6 | 1.438 | 0.041 2 |
|      |       | C 2p | 0.830 74 | 0.368 1 | 0.558 |
|      |       | O 2p | 1.030 692 | 0.194 326 | 1.114 2 |
|      |       | F 2s | 0 | 0 | 0.129 326 |
|      |       | F 2p | 0.174 968 | 0 | 0.157 28 |
| 75   | 16.643 | C 2s | 0.315 8 | 1.062 678 | 0.358 8 |
|      |       | C 2p | 0.820 52 | 0.456 4 | 0.697 8 |
|      |       | O 2p | 0.726 6 | 0.239 2 | 0.785 |
|      |       | F 2s | 0 | 0.033 6 | 0.058 |
|      |       | F 2p | 0.421 29 | 0.208 24 | 0.423 4 |
| 74   | 17.461 | C 2s | 0.162 078 | 1.271 231 | 0.114 2 |
|      |       | C 2p | 0.577 231 | 0.341 6 | 0.529 6 |
|      |       | O 2p | 0.112 333 | 0.027 14 | 0.114 2 |
|      |       | F 2s | 0 | 0.012 2 | 0 |
|      |       | F 2p | 1.148 298 | 0.348 | 1.292 2 |
| 73   | 18.004 | C 2s | 0.248 341 | 1.248 341 | 0.023 2 |
|      |       | C 2p | 0.487 808 | 0.399 6 | 0.548 4 |
|      |       | O 2p | 0.347 846 | 0.071 86 | 0.378 6 |
|      |       | F 2p | 0.914 803 | 0.282 | 1.049 8 |
| 72   | 18.614 | C 2s | 0.089 677 | 0.976 277 | 0.063 4 |
|      |       | C 2p | 0.494 8 | 0.481 66 | 0.389 |
|      |       | O 2p | 0.306 484 | 0.090 54 | 0.338 4 |
|      |       | F 2s | 0 | 0.011 96 | 0.005 8 |

FIG. 5. Molecular cross section of CgF12O (weighting factor in Refs. 12 and 13).

IV. CONCLUSION

In this paper, the total cross section of electron-impact ionization of CgF12O molecules is calculated by the DM formula. In the calculation of the atomic orbital composition of the molecule, two different methods, the addition base function and the NAO, are used and the basis function distribution is based on MPA and SCPA. The cross sections are calculated for H2O, CsH4O, CsF6O, and CgF12O using three different methods. At the same time, the effects of the atomic orbital weight factor are compared.

For the H2O molecule, the calculated values obtained by the SCPA and NAO methods are in good agreement with the measured values. For the CsH4O molecules, the calculated values obtained by the three methods using the modified weight coefficients are not much different. For the macromolecular CsF6O and CgF12O molecules, the modified weight factor has little effect on SCPA and the calculated value is significantly higher than the other two calculation methods. It seems more reasonable to use the MPA and NAO methods. In the absence of measured values, the calculation results in this paper can provide a basis for the calculation of the electron swarm parameter in the CgF12O gas discharge process, so as to deeply evaluate the feasibility of the application of the gas in electrical equipment.

ACKNOWLEDGMENTS

This work was supported by the National Natural Science Foundation of China (Program No. 51707137) and the China Scholarship Council.

REFERENCES

1. X. Li, H. Zhao, and A. B. Murphy, ‘‘SF6-alternative gases for application in gas-insulated switchgear,’’ J. Phys. D: Appl. Phys. 51(15), 153001 (2018).
2. D. Chen, X. Zhang, H. Xiong et al., ‘‘A first-principles study of the SF6 decomposed products adsorbed over defective WS2 monolayer as promising gas sensing device,’’ in IEEE Transactions on Device and Materials Reliability (IEEE, 2019).
3. Y. Wu, C. Wang, H. Sun et al., ‘‘Evaluation of SF6-alternative gas C5-PFK based on arc extinguishing performance and electric strength,’’ J. Phys. D: Appl. Phys. 50(38), 385202 (2017).
4. Y. Li, X. Zhang, S. Tian, S. Xiao et al., ‘‘Insight into the decomposition mechanism of CsF6O-CO2 gas mixture,’’ Chem. Eng. J. 360, 929–940 (2019).
5. S. Tian, X. Zhang, S. Xiao et al., ‘‘Experimental research on insulation properties of CsF6O/N2 and CsF6O/CO2 gas mixtures,’’ IET Gener., Transm. Distrib. 13(3), 417–422 (2018).
6. Y. Kieffel, T. Irwin, P. Ponchon et al., ‘‘Green gas to replace SF6 in electrical grids,’’ IEEE Power Energy Mag. 14(2), 32–39 (2016).
7. S. Tian, X. Zhang, S. Xiao et al., ‘‘Application of CsF6O/CO2 mixture in 10 kV medium-voltage switchgear,’’ IET Sci., Meas. Technol. 13(9), 1225–1230 (2019).
8. S. Tian, X. Zhang, Y. Wang et al., ‘‘Partial discharge characteristics of CsF6O/CO2 mixed gas at power frequency AC voltage,’’ AIP Adv. 9(9), 095057 (2019).
9. X. Zhang, Y. Wang, Y. Li et al., ‘‘Thermal compatibility properties of CsF6O-air gas mixture with metal materials,’’ AIP Adv. 9(12), 125024 (2019).
10. X. Zhang, S. Tian, S. Xiao et al., ‘‘Insulation strength and decomposition characteristics of a CsF6O and N2 gas mixture,’’ Energies 10(8), 1170 (2017).
11. X. Yu, H. Hou, and B. Wang, ‘‘Prediction on dielectric strength and boiling point of gaseous molecules for replacement of SF6,’’ J. Comput. Chem. 38(10), 721–729 (2017).
H. Deutsch, K. Becker, S. Matt et al., “Theoretical determination of absolute electron-impact ionization cross sections of molecules,” Int. J. Mass Spectrom. 197(1-3), 37–69 (2000).

J. Xiong, X. Li, J. Wu et al., “Calculations of total electron-impact ionization cross sections for fluoroalkanes C\textsubscript{2}F\textsubscript{2}O and fluoronitriles C\textsubscript{2}F\textsubscript{2}N using modified Deutsch–Märk formula,” J. Phys. D: Appl. Phys. 50(44), 445206 (2017).

Y. K. Kim and M. E. Rudd, “Binary-encounter-dipole model for electron-impact ionization,” Phys. Rev. A 50(5), 3954–3967 (1994).

Y. K. Kim, J. Paulo Santos, and F. Parente, “Extension of the binary-encounter-dipole model to relativistic incident electrons,” Phys. Rev. A 62(5), 052710 (2000).

Y. K. Kim, W. Hwang, and M. E. Rudd, “New model for electron-impact ionization cross sections of molecules,” J. Chem. Phys. 104(8), 2956–2966 (1996).

L. Zhong, J. Wang, X. Wang et al., “Calculation of electron-impact ionization cross sections of perfluoroketone (PFK) molecules C\textsubscript{x}F\textsubscript{2x}O (x = 1-5) based on binary-encounter-Bethe (BEB) and Deutsch-Märk (DM) methods,” Plasma Sources Sci. Technol. 27, 095005 (2018).

L. Zhong, J. Xu, X. Wang, and M. Rong, “Electron-impact ionization cross sections of new SF\textsubscript{6} replacements: A method of combining binary-encounter-Bethe (BEB) and Deutsch-Mark (DM) formalism,” J. Phys. D: Appl. Phys. 50(44), 445206 (2017).

R. Carbó-Dorca and P. Bultinck, “Quantum mechanical basis for Mulliken population analysis,” J. Math. Chem. 36(3), 231–239 (2004).

R. Margreiter, H. Deutsch, and T. D. Märk, “A semiclassical approach to the calculation of electron impact ionization cross-sections of atoms: From hydrogen to uranium,” Int. J. Mass Spectrom. Ion Processes 139, 127–139 (1994).

H. Deutsch, K. Becker, R. Basner et al., “Application of the modified additivity rule to the calculation of electron-impact ionization cross sections of complex molecules,” J. Phys. Chem. A 102(45), 8819–8826 (1998).