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Geometry of Ozone Molecule

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Abstract: *Geometry of ozone molecule is discussed.*

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1. Introduction

We will pay attention to the geometry of ozone molecule consisting of three oxygen atomswhich express two kinds of mutual distance: the shorter$from\ O^+to\ O^-$and the longer one$from\ O^-to\ O^-$ as shown in Figure 1:

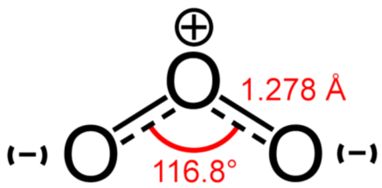

Figure1. *The ozone molecule*

Applying data from reference [1] and taking into account wave restrictions the exact geometry on the double surface should be found with the help of key formulasthat relate the length on the elliptic surface $n$to the length on the average elliptic-hyperbolic surface $s(n)$ as follows[2]:

$$s(n) = n\left(2 - \frac{1}{\sqrt{1+\frac{\pi^2}{n^2}}}\right). \tag{1}$$

As well as the length on the elliptic surface $n$to the length on thehyperbolic surface $h(n)$as follows[3]:

$$h(n) = n\left(2\sqrt{1+\frac{\pi^2}{n^2}} - 1\right). \tag{2}$$

2. Subtle Bonding between Oxygen Atom $O^+$and OxygenAtom O^-in Ozone MoleculeO_3

The shorter distance$d_{O^+O^-\ in\ O_3}^{measured}$measured between the oxygen atom $O^+$and the oxygen atom O^- in the ozone molecule$O_3$is long$127.80\,pm = 52.673\ \lambda_e$[1].The πtimes longer orbit of$s_{O^+O^-\ in\ O_3}^{measured} = 165{,}476\ \lambda_e$ is close to the geometrically unstableorbit $s(165.5\ \lambda_e) = 165.560\ \lambda_e$.(1)But the doubled value $2s_{O^+O^-\ in\ O_3}^{measured} = 330.952\ \lambda_e$ is close to the geometrically stable orbit $s(331\ \lambda_e) = 331.015\ \lambda_e$(1). So, it shows that the stable subtle bonding orbit O^+O^-between oxygen atom $O^+$and oxygen atom O^-in ozone molecule $O_3$is formed.

3. Subtle Anti-Bonding Orbits between Oxygen Atom $O^+$and Oxygen Atom O^-in Ozone MoleculeO_3

The stable doubled subtle bonding orbit between oxygen atoms of elliptic length $2n_{O^+O^-} = 331\lambda_e$can be equally divided to two unstable doubled anti-bonding orbits of elliptic length $2n_{O^+} = 2n_{O^-} = 165.5\ \lambda_e$. But they can bypass the geometric instability by yin yang trick [3] where the electron wave retreats to an adjacent orbit before annihilating in the native orbit.We just have to take into account that subtle anti-bonding orbits are energetically less favourable than is the bonding orbit so the input of energy is needed for their formation[4]:

$$\Delta E_{forming}^{anti-bonding} = Ry.\alpha^{-1}\left(-\frac{1}{s\left(\frac{n_{O^+O^-}}{2}\right)}+\frac{1}{\frac{s(n_{O^+O^-})}{2}}\right). \quad (3a)$$

Where in our case $n_{O^+O^-} = 165.5\,\lambda_e$is available. Then applying $Ry = 13.605\,693\,009\,eV$ as well as $\alpha^{-1} = 137.035\,999\,146$ and inserting needed data the next result is given:

$$\Delta E_{forming}^{anti-bonding} = 0{,}0121\,508\,eV. \quad (3b)$$

Energy 0.012 eV allows permutation of oxygen atoms in ozone.[5]

4. Subtle Bonding between two Oxygen Atoms O^- in Ozone Molecule O_3

The longerdistance $d_{O^-O^-\,in\,O_3}^{measured}$measured between two oxygen atomsO^-in the ozone molecule $O_3$is long $217.70\,pm = 89.725\,\lambda_e$ [1].The πtimes longer orbit of$s_{O^-O^-\,in\,O_3}^{measured} = 281.879\,\lambda_e$is nearbythe geometrically unstable orbit$s(281.5\,\lambda_e) = 281.518\,\lambda_e$. (1)Andthe doubled value $2s_{O^-O^-\,in\,O_3}^{measured} = 563{,}757\,\lambda e$ is also nearby the geometrically unstable orbit$s(563.5\lambda e)=563.509\,\lambda e$.(1) So, it shows that the stable subtle bonding orbit O^-O^-between two oxygen atomsO^-in ozone molecule O_3 is not formed.

5. Subtle Anti-Bonding Orbits between Oxygen Atoms O^- in Ozone Molecule O_3

The unstable doubled subtle bonding orbit between oxygen atoms of elliptic length $2n_{O^-O^-} = 563.5\lambda_e$can be equally divided to two unstable doubled anti-bonding orbits of elliptic length $2n_{O^-} = 2n_{O^-} = 281.75\,\lambda_e$. They can bypass the geometric instability by yin yang trick [3]where the electron wave retreats to an adjacent orbit before annihilating in the native orbit. We just have to take into account that subtle anti-bonding orbits are energetically less favourable than is the bonding orbit so the input of energy is needed for their formation[4]:

$$\Delta E_{forming}^{anti-bonding} = Ry.\alpha^{-1}\left(-\frac{1}{s\left(\frac{n_{O^-O^-}}{2}\right)}+\frac{1}{\frac{s(n_{O^-O^-})}{2}}\right). \quad (4a)$$

Where in our case $n_{O^-O^-} = 281.75\,\lambda_e$is available. Then applying $Ry = 13.605\,693\,009\,eV$ as well as $\alpha^{-1} = 137.035\,999\,146$ and inserting needed data the next result is given:

$$\Delta E_{forming}^{anti-bonding} = 0{,}002\,466\,307 eV = 0{,}0025\,eV. \quad (4b)$$

Thefrequency equivalent of the above energyyields596 GHz andozone has absorption peaks in this frequency range. [6]

6. The Exact Geometry of Ozone Molecule

Respecting present theoretical approach an exact geometry of ozone molecule can be offeredon the chosen basis. The results are collected in Table1.

Table1. *Exact values of oxygen orbit lengths and angle between oxygen atoms in ozone molecule on different surfaces*

Ellipticorbit length	**Averageelliptic-hyperbolic orbit length**	**Hyperbolicorbit length**
$n_{O^+O^-} = 165.\mathbf{50}\,\lambda_e$	$s(n_{O^+O^-}) = 165.\mathbf{529}\,809\,\lambda_e$	$h(n_{O^+O^-}) = 165,\mathbf{559}\,630\,\lambda_e$
$n_{O^-O^-} = 281.\mathbf{75}\,\lambda_e$	$s(n_{O^-O^-}) = 281.\mathbf{767}\,513\,\lambda_e$	$h(n_{O^-O^-}) = 281,\mathbf{785}\,029\,\lambda_e$
Ellipticangle	**Average elliptic-hyperbolic angle**	**Hyperbolic angle**
$\varphi_{O^-O^+O^-} = 116,\mathbf{686}\,705°$	$\varphi_{O^-O^+O^-} = 116,\mathbf{664}\,789°$	$\varphi_{O^-O^+O^-} = 116,\mathbf{64}2\,877°$

Curved distances are given with the help of equations (1),(2), and angles using cosine rule (5)

$$cos\varphi_{O^-O^+O^-} = 1 - \frac{1}{2}\left(\frac{(O^-O^-)}{(O^+O^-)}\right)^2. \quad (5)$$

Differences in geometry with respect to the applied surface are noticeable to the second decimal place.

7. Conclusion

There is no exact geometry in general. As long as two geometries are available we can talk only about exact values on the elliptic or hyperbolic and consequently average elliptic – hyperbolic surface.

Dedication

To ozone as the umbrella of the Earth

Figure2. *The umbrella of the Earth*

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