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APPLICATION OF PARTICLE-IN-A- RING MODEL TO PREDICT THE MAXIMUM ABSORBANCE (Λ_{MAX}) OF CORONENE

***Jayprakash S. Chauhan**

Department of Chemistry, C.U. SHAH Science College, Nr. Gujarat University, Ashram Road, Ahmadabad. Gujarat, India.

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***Corresponding Author**
Jayprakash S. Chauhan
Department of Chemistry, C.U. SHAH Science College, Nr. Gujarat University, Ashram Road, Ahmadabad. Gujarat, India.

ABSTRACT

Coronene is known as super benzene. This molecule is characterized by a big cloud of delocalized electrons spread over the entire surface of molecule. This has attracted a lot of interest in its research. The other peculiarity of this molecule is that it emits blue light in presence of UV radiation. This molecule contains alternate double bonds. The electron cloud or electrons are assumed to move around the peripheral region of the molecule is considered to be forming a ring like structure. We have made an effort to apply the quantum mechanical model – 'Electron in a Ring' to predict the UV/VIS absorption peak [λmax] of the molecule. The result roughly agrees with the experimental observation with 31 ٪ error. Discussion focuses on how the electron on a ring model works, the assumptions that are made, its limitations, causes of error and its uses. This model may be used to bridge theoretical and experimental results.

KEYWORDS: Coronene, electron in a ring model, delocalization, assumptions, absorbance.

INTRODUCTION

The quantum mechanical models such as particle in a box and particle in a ring have been used to understand the nature of molecules and atomic particles. The equation can be used to predict how electrons move over large molecules and move across conjugated double bonds. The equation for electron in a ring model works effectively by assuming that an electron moves around the circular track with constant potential energy. The solution of the Schrodinger equation gives Eigen values which are characterized by quantum states. The particle in a ring model has been used as teaching application of molecules such as Azulene.[1] The electronic energy levels of Polyacenes have been calculated by the electron in

a ring model.[2] New teaching methods have been developed for electron in a ring model using cyclic Polyenes.[3] The PIB model and the electron in a ring model have been used to interpret the UV-VIS spectra of linear conjugated Polyenes and Annulenes.[4,5] A simple free electron model and modification of this model has been described by Gerhard Taubmann.[6] Similarly Jochen Autsch batch has used particle in a box model to predict the λmax and other properties of cyanine dyes.[7] Gion calzaferri has used PIB model for the description of few of the conjugated systems.[8] The structure of β-carotene and lutein has been studied with reference to PIB model and experiment has been devised by Henery, Anderson & Todd wimpfhimer.[9,10]

Coronene is a polycyclic aromatic hydrocarbon – (PAH). It is made up of six fused benzene rings. This compound is also known as super-benzene. Its chemical formula is $C_{24}H_{12}$. It is a yellow material that dissolves in solvents such as benzene, toluene, ethanol etc. This compound has a planar structure with seven carbon rings and posses D_6h point group. It occurs naturally as mineral carpathite. It is also found as one of the pollutants in the environment. This compound is aromatic but the Huckel rule is not obeyed.

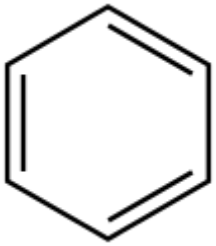
Coronene is characterized by its delocalized electrons. The electron density is centered over the peripheral region. We have assumed that it forms a ring like structure. For this reason, the electron in a ring model has been applied. It has been reported that its ethanolic solution gives λmax at 302 nm (extinction – 16650) which has been considered for the comparison.[11] Its spectra depend on the solvent.[11]

MATHEMATICAL METHODS

The π- electrons of Coronene are considered to form a circular track, where length of circumference of the ring is contributed by the carbon skeleton. As an illustrative example, we have calculated the λmax of benzene. The following steps or assumptions are important for molecules having ring like structure where this model may be applied.

1. Add the C – C bond length to get the circumference of the ring. Generally we use average C – C bond length as 1.39 $x10^{-8}$ cm. We assume that the π electrons are free to move approximately on or around the circular track or ring. The length of the ring is calculated as (N) x 1.39 x 10^{-8} cm where N is the no. of bonds in the skeleton.
2. Each π - bond will contribute 2 electrons.
3. Each of the energy level of the ring can occupy maximum of two electrons.

4. Let us take a simple example of Benzene. The circumference of this molecule as per our assumption, (N) x 1.39x 10^{-8} will be 6 x1.39 x10^{-8} = 8.34x10^{-8}cm =0.834 nm.



The energy of an electron moving in a ring can be obtained by solving the Schrodinger equation which can be represented as $E = n^2h^2/2ma^2$ where n= *0, ±1, ±2….α,* h= *Planck's constant,* m= *mass of* electron, a = length of circumference of the ring.

The first and the second energy level occupy the two and four electrons respectively. The highest occupied level (i.e. $E_1 = h^2/2ma^2$) can absorb radiation and can be excited to the 3Π level.

n=2 ----------. 3Π

n=1 --↑↓---, --↑↓---. 2Π

n =0 ---↑↓----------. 1Π

Energy levels of benzene

$\Delta E = E_2 - E_1 = 4h^2/2ma^2 - 1h^2/2ma^2 = 3h^2/2ma^2$

We know that $\Delta E = \frac{hc}{\lambda}$

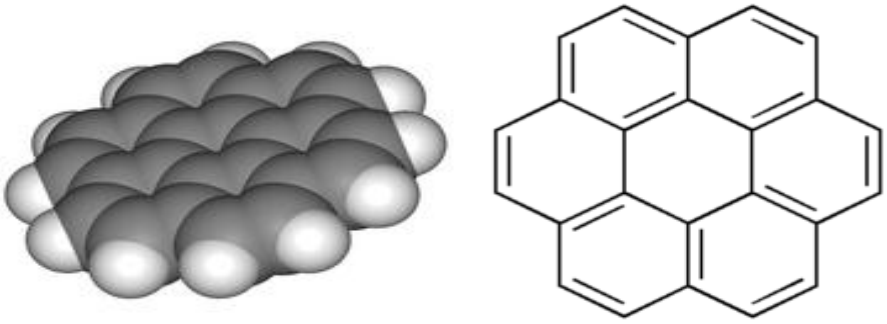
Therefore $\lambda = hc/\Delta E = 2mca^2/3h$.

Inserting the value of Planck's constant h =6.632 x 10^{-27}erg s., mass of electron=9.11 x 10^{-28} gms., C – velocity of light = 3.00 x 10^{10} cm/s, 'a' – the length of circumference of the ring = 8.34 x 10^{-8}cm, the value of λmax can be calculated.

For this system the λmax calculated comes to be, λcal. = 194 nm

λ-experimental is the actual λmax obtained from the experimental results. The experimental value of this compound λexpt. is 254 nm.

We have followed the same method in the study of Coronene by use of electron in a ring model.



Structure of Coronene.

The following Table-1 illustrates the experimental λmax, calculated λmax using electron in a ring model, the error in the value of λmax and the % relative error.

Table: 1.

Coronene	Double bonds n	λ_{max} expt. nm	λ_{max} cal nm	Error in nm	% error
$C_{24}H_{12}$	12	302	397	95	31

Causes of the error

From the result shown in the above table it seems that the error in the calculated result arises due to the delocalization of electrons over the entire peripheral region. Delocalization may cause alterations in the bond length. The wavelength- λ is sensitive to the circumference of the ring. Due to the delocalization, it seems that there is a decrease in the C-C bond length. There is a shrinkage in the length- 'a' as there develops a partial double bond between each carbon atom in the chain and we suppose that the electron cloud moves over the entire ring in such a way that it leads to the reduction in the circumference of the entire ring. But, as per our assumptions we have fixed the distance between the carbon atoms. Thus in order to minimize the error, we must reduce the distance between carbon atoms. This discussion is strictly as per the electron in a ring model. Following table illustrates how this can be achieved.

Table: 2.

Bond length C-C A^0	λexpt nm	λcal nm	Error nm	⁒Error
1.39	302	397	95	31
1.38	302	391	89	29
1.36	302	380	78	25
1.34	302	369	67	22
1.32	302	358	56	18
1.30	302	347	45	14
1.28	302	337	35	11

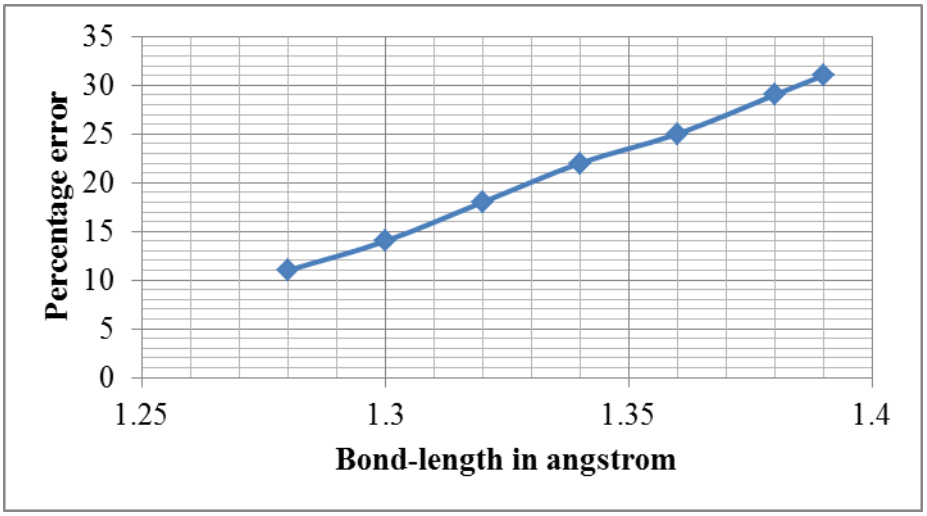


Fig-1. Percentage error verses the bond length.

We can observe from the graph that in order to minimize the error, shorter bond length is supposed to be assumed.

CONCLUSION

The electron in a ring model has been used to predict the λmax of the Coronene. The result obtained by the use of electron in a ring model indicates that the error in the determination of maximum absorbance is around 31% for Coronene. The cause of the error is due to the fact that we have fixed the value of length of the circumference by our assumptions and potential energy is considered as constant. The bond alterations are common in such molecules. It is also reported that the maximum absorbance of Coronene depends on the type of solvent. We have made an effort to interpret only one maxima obtained in ethanolic solution at 302 nm (molar extinction- Ɛ=16000).[11] Other peaks obtained in the UV / VIS spectrum cannot be interpreted by our simple electron in a ring model. This may be used as a rough exercise for the application of electron in a ring model.

Applications of Coronene

Coronene is an electron rich compound. It can form a strong complex with explosive materials which are electron deficient nitro aromatics. This has shown that Coronene micro wires may be used for detection of explosives.[12] Light emitting behaviors of Coronene nanowires have been investigated recently.[13] Coronene in solid form can function as electrode material with characteristics of dual ion batteries.[14] Coronene has been used as a solvent probe.[15] Super conducting material has been devised using metal trapped Coronene compounds.[16]

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REFERENCES

1. Miguel A.R. B. Castanho; *Journal of chemical education*; 2002; 79(9).
2. Gantaro Araki; *Prog. Ther. Phys.*, 1956; 16(4): 265-268.
3. Bruce D. Anderson; *J. Chem. Educ*. 2012; 89(6): 724-727.
4. J.S. Chauhan, R.P.Patel,; *Der pharma chemica*, 2016; 8(5): 67-73.
5. J. S. Chauhan, A. V. Pandya ; WJPR, 2016; 5(11): 428-435.
6. Gorter S.i. Rutten, E.i. Krever, M. I. Romers, D.W.J., [18] *Acta. Crystallogr*. B, 1995; 51: 1036-1045.
7. Jo Chen Autschbach, *J. Chem. Educ*., 2007; 84(11): p-1840.
8. Separat druck qus, *CHIMIA* 41, Nr. 7-8 (July-August), p-248-250, 1987
9. Particle in box- lab experiment, *journal of Laboratory chemical Education*. 2015; 3(2): 19-21.
10. Henery, M. Roth H. and Anderson, the Particle in a box redux; *J. Chem. Educ*., 2012; (89): 960-961.
11. Studies of Properties of Coronene in solution; Furat Bayrakceken and Ali Umit Keskin; Yeditepe University, *Dept. of Electrical Engineering*, Kayrsdagi-34755, Istanbul, Turkey.
12. Hong Wang, xiao-He xu, Hai-Fengji, *Nanotechnology Development* – volume-2, issue-1, 2012.
13. Jinchong xiao, Huiving Yang; *Journal of mater, chem*., 2011; 21: 1423-1427.
14. Ismael A. Rodriguez-Perez, Zelang jian, *ACS Energy Lett*. 2016; 1(4): 719-723.
15. Waris R., Rembert MA, The Analyst, 1989; 114(2): 195-199.
16. Yoshihiro Kubozono; *Chem. Phys*., 2011; 13(37).