Quick Calculation of Sigma and Pi Bonds

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Abstract

The research file is mainly aimed to provide chemists with a useful theoretical technique for the calculation of sigma and pi bonds_even in the most complex molecule (except in the co-ordination molecule). The all, we need to know the molecular formula along with the number of rings and bonds formed by some exceptional elements. Here exceptional means those atoms which show multiple valencies.

The research paper consists of the derivation of the formulae and a conversion chart helping in calculating the number of pi bonds. The formulae is solely derived by me and thus the research file is uniquely original.

The basic structure of the formulae is-

In any $A_aB_bC_c$.... type molecule the number of σ bonds is: (a+b+c+....)+ n(R)-1

and the number of π bonds in C_aH_b type molecule is: a-b/2-n(R)+1.

In the compounds other than pure hydrocarbons the number of π bonds is calculated with the help of conversion chart prepared in the research work.

Keywords: sigma bonds, pi bonds, conversion chart, useful formulae

Introduction

Chemistry is very useful in our day-to-day life and our chemists are working a lot to make it more useful. They try to explain the physical and chemical properties of various compounds with the help of their molecular structures. One of the very important features of these compounds' molecular structure is the number of different types of bonds that help in the determination of a lot of characteristics.

The total number of electron sharing bonds= number of σ bonds + number of π bonds.

What is a sigma bond?

Sigma Bond[1]: "Sigma bond is a covalent bond formed by the overlap of atomic orbitals and/or hybrid orbitals along the bond axis (i.e., along a line connected the the 2 bonded atoms.)"

Pi Bond[2]: The bond formed between 2 atoms by the sideways overlapping of 2 orbitals is called pi bond.

Objective of Study

To find general formulae for quick calculation of σ and π bonds.

Hypothesis or Principle Proposed

The number of σ and π bonds in a molecule depends upon the number of the different-different atoms in its molecular formula, number of rings in the molecule and number of bonds formed by exceptional elements (i.e.,the elements which show multiple valencies).

Principle Involved

- Alkanes (C_aH_{2a+2}) and Cycloalkanes (CaH2a) have zero pi bonds.

Observations

1. When 1 pi bond forms, 2H from alkane or cycloalkanes reduce.
2. In open chained compounds 1^{st} carbon is not bonded with the last one but in ringed compounds, 1^{st} carbon is bonded with the last one.
3. When 2 rings are combined, with respect to the lack of 2C, there is one σ bond reduced, in this case 2C and 6H reduce means $-CH_2-CH_2-$ and 2H (1π bond) reduce.

Conclusive Formulae

Let's consider 2 types of conditions through which we will reach till general formulae:

Condition I

When number of rings n(R)=0 i.e., compound is open chained, then

Number of σ bonds= a+b-1 {Observation -2}

Number of π bonds= (2a+2-b)/2 {Observation -1 and principle involved}

Condition II

When number of rings n(R)= 1,

then the number of σ bonds = a+b {Observation-2}

Number of π bonds= (2a-b)/2= a-b/2 {Principle involved and observation- 1}

Now, we can generalise the formulae on the basis of observation-3.

As we knew that when one ring is combined with an existing ring, 1 sigma bond increases and 1 π bond reduces, then generally-

Number of sigma bonds in a C_aH_b type molecule= **a+b+n(R)-1** ......(1)

The factor -1 is due to the existing one ring.

Similarly, the number of π bonds= **a-b/2-n(R)+1** ......(2)

Equation (1) and (2), both satisfies the condition 1 & 2 proved earlier.

Now, you would be thinking that this formula set is only applicable for pure hydrocarbons, but it's not the exact case.

First of all through eq^n (1) we can generalise the formula for the calculation of sigma bonds:

The number of sigma bonds in a $A_aB_bC_c$ .... type molecule is (a+b+c+....)+n(R)-1.

So, by now we have completed an important task and that is the calculation of sigma bonds in any molecule, knowing just the number of rings along with the molecular formula.

There's a generalisation method prepared by me even for the calculation of π bonds. The generalisation method is prepared with the help of **Equivalence Concept** again proposed by me.

This concept helps us building a C-H based system that is useful in the calculation of π bonds.

Equivalence Concept

This concept is only applicable for the calculation of π bonds. We have a way of calculating π bonds in C_aH_b type molecule but what if, we had a way that convert all molecule into C_aH_b type and that is whereby this concept is applied.

Through this concept, we convert all other elements except C and H like O, N, B, S etc. into C_aH_b form, more specifically CH_b form

The mind map of the concept is as follows:

Bonds Formed by the Element in the molecule = 4(1)-1(b)= 4-b {through CH_b form}

Example:

We know that **O forms 2 bonds** very commonly, when it forms 2 bonds (assume CH_3COOH), then, 2= 4-b, b=2, thus we get CH_2 from O, i.e., O will be replaced with CH_2. Thus, now the molecular formula is $CH_3C(CH_2)_2H$ or C_4H_8.

No. of π bonds in C_4H_8= 4-8/2-0+1= 1, and we know that there's 1 π bond in CH_3COOH.

Note: We can even neglect CH_2as $-CH_2-$ has 0 π bonds.

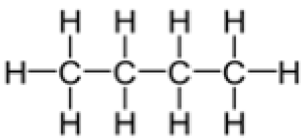
Neglecting O in CH_3COOH, we get molecular formula as C_2H_4 and the number of π bonds= 2-4/2-0+1= 1

Now, here is the conversion chart made from above discussion for different- different elements.

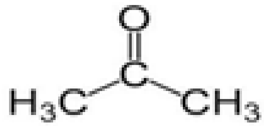
Bonds Formed Considered	Conversion	Example Elements
1	CH_3 or H	Na, Li etc. in their common chlorides(NaCl, LiCl etc.)
2	CH_2 or neglect	Be, Mg, etc. in their common oxides or chlorides
3	CH	B, Al, etc. in their common chlorides
4	C	Si, Ti etc. in their common chlorides
5	CH_{-1}	P, N in PCl_5, HNO_3
6	CH_{-2}	S in H_2SO_4, Schiff's reagent and Mn in K_2MnO_4
7	CH_{-3}	Mn, I in $KMnO_4$, IF_7
8	CH_{-4}	Xe in $(XeO_6)^{-4}$ ion

Examples:

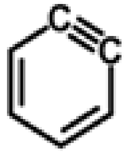
Butane (C_4H_{10}) [3]:
No. of σ Bonds in C_4H_{10}= a+b+n(R)-1= 4+10+0-1= 13
No. of π Bonds in C_4H_{10} = 4-5-0+1= 0



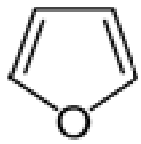
Acetone (C_3H_6O) [4]:
No. of σ Bonds in C_3H_6O= 3+6+1-1= 9
No. of π bonds= 3-3-0+1=1



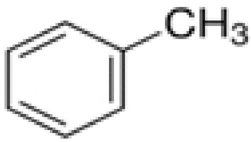
Benzyne (C_6H_4) [5]:
σ bonds in C_6H_4= 6+4+1-1= 10
π bonds = 6-4/2-1+1= 4



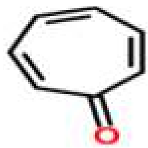
Furan (C_4H_4O) [6]:
No. of σ bonds in Furan= 4+4+1+1-1= 9
No. of π bonds = 4-4/2= 2



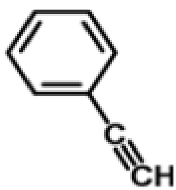
Toluene (C_7H_8) [6]:
σ bonds in C_7H_8= 7+8+1-1= 15
π bonds= 7-4-1+1= 3



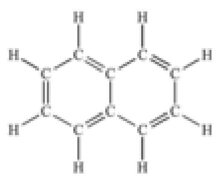
Tropone (C_7H_6O) [8]:
No. of σ bonds in tropone= 7+6+1+1-1=14
No. of π bonds in tropone= 7-6/2-1+1= 4



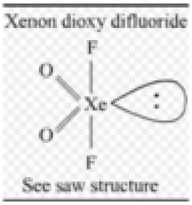
Phenylacetylene (C_8H_6) [9]:
σ bonds= 8+6+1-1= 14
π bonds= 8-6/2-1+1= 5



Naphthalene ($C_{10}H_8$) [10]:
No. of σ bonds = 10+8+2-1= 19
No. of π bonds = 10-8/2-2+1= 5
Here, no. of rings n(R)= 2



Xenon Dioxydifloride (XeO_2F_2) [11]:
No. of σ bonds in XeO_2F_2 = 1+2+2-1= 4
As the total bonds formed by Xe, O and F= 6, 2 and 1.
Changed form = $CH_{-2}H_2$= C
Number of π bonds = 1-0/2-0+1= 2



Calcium Carbide (CaC_2) [12]:
No. of σ bonds in CaC_2 = 1+2+1-1= 3
As Ca forms 2 bonds and that is why can be neglected.
So number of π bonds= 2-0-1+1= 2

Application of The Formulae

- In the calculation of the degree of unsaturation.
- Quickly dealing with macro-molecules where number of rings n® is known.
- Rough idea about the hybridization.
- In having the idea of relative strength of molecules.

Conclusion

Thus the derived formula set helps us calculate the number of sigma and pi bonds in a molecule in quick manner and that is why the research paper is entitled as 'Quick Calculation of Sigma and Pi Bonds'. I hope that the formula set will help chemists for their theoretical work and hereby the deducted hypothesis is confirmed that the number of sigma and pi bonds in a molecule depends upon the number of atoms and rings in it along with the number of rings. In some doubtful cases, we also consider bonds formed by a distinct atom (as most of the time it is known to us).

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