

A Rapid and Innovative Method for the Identification of Aromatic and Anti-aromatic Nature of Organic Compounds

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Abstract Prediction of aromatic and anti-aromatic behavior of organic compounds is a vitally important tool for students of chemistry at graduate and post-graduate level for solving different kinds of problems regarding reactivity, stability and acidic properties etc. In this manuscript we try to present a simple and innovative method for easy identification of aromatic and anti-aromatic behavior of organic compounds from their non-aromatic nature excluding Huckel's rule of aromaticity.

Keywords: planar, cyclic system, number of π bonds, delocalized electron pair, negative charge, even no and odd no

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1. Introduction

The method which is generally used [1,2,3,4] for the prediction of aromatic and anti-aromatic nature of organic compounds based on Huckel's rule of aromaticity is time consuming and confusing. Keeping this in view, an innovative method is necessary for the identification of aromatic and anti-aromatic nature of organic compounds from their non-aromatic nature.

Earlier seven new innovative methods including ten new formulae are introduced on the easy prediction of 'Bond-Order of mono and diatomic homo and heteronuclear molecules or ions', 'Bond-order of oxide based acid radicals', 'Hybridization', 'IUPAC nomenclature of spiro and bicyclo compounds', 'spin multiplicity value calculation and prediction of magnetic properties of diatomic hetero nuclear molecules and ions [5,6,7,8,9].

The present study will be a new innovative method involving two formulae by just manipulating the no of π bonds within the ring system and delocalized electron pair (excluding π electron pair within the ring system) with one (01). It would go a long way to help the students of organic chemistry who would choose the subject as their carrier. Experiment *in vitro* on 100 number of students show that the prediction of aromatic and anti-aromatic behavior of different kinds of organic compounds using Huckel's rule, strike rate is 1Q/3min and by using these new innovative methods strike rate is 1Q/30secs.

On the basis of this, we can strongly suggest that by using this method the students can identify the aromatic and anti-aromatic nature of different kinds of organic compounds from their non-aromatic nature in a very short interval of time.

2. Discussion

2.1. Prediction of Aromatic Behavior

In the first case, the compound must be cyclic, planar (i.e. all the carbon atoms having same state of hybridization) with even number of A value, where $[A = \pi b + e^p + 1$ (constant)], here πb = number of π bonds with in the ring system and e^p = number of electron pair outside or adjacent to the ring system i.e. if the ring contains hetero atoms (atoms containing lone pair of electrons) which can undergo delocalization and each negative charge if present may be treated as one pair of electrons.

If the value of 'A', for a certain organic compound comes out as even number then this compound will be treated as aromatic compound.

2.2. Prediction of Anti-aromatic Behavior

In the second case, the compound must be cyclic, planar (i.e. all the carbon atoms having same state of hybridization) with odd number of A value, where $[A = \pi b + e^p + 1$ (constant)], here πb = number of π bonds with in

the ring system and e^-p = number of electron pair outside or adjacent to the ring system i.e. if the ring contains hetero atoms which can undergo delocalization and each negative charge if present, may be treated as one pair of electrons.

If the value of 'A', for a certain organic compound comes out as odd number then this compound will treat as anti-aromatic compound.

2.3. In General Condition for Non-aromatic Behavior of Organic Compounds

Any compound that lacks one or more of the above features i.e. it may be acyclic / non-planar, is to be treated as non aromatic. But in this case, 'A' value may be even or odd number.

It is always to be noted that if the ring contains hetero atom like N, O, S etc, in this case we must count that electron pair in the evaluation of 'A' value which can undergo delocalization. We never count localized electron pair.

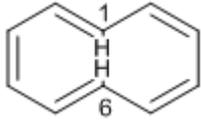
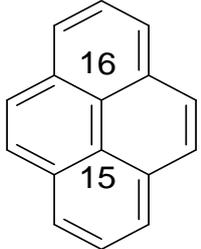
Examples are presented in [Table 1](#).

Table 1. (Aromatic, anti-aromatic and non-aromatic nature of organic compounds by calculating A value)

Organic Compound (Cyclic, Planar/Cyclic, non-planar)	πb value [πb = number of π bonds with in the ring system]	e^-p value [e^-p = number of delocalized electron pair outside or adjacent to the ring system]	A value [$A = \pi b + e^-p + 1$ (constant)] (even no/odd no)	Nature of compound (aromatic/anti-aromatic/non aromatic)
Benzene or [6] annulene (Cyclic, Planar)	3 π bonds	0	3 + 0 + 1 = 4 (even no)	Aromatic
Naphthalene (Cyclic, Planar)	5 π bonds	0	5 + 0 + 1 = 6 (even no)	Aromatic
Anthracene (Cyclic, Planar)	7 π bonds	0	7 + 0 + 1 = 8 (even no)	Aromatic
Cyclopropene (Cyclic, non planar due to one sp^3 hybridized carbon atom)	1 π bond	0	1 + 0 + 1 = 2 (even no)	Non-aromatic
Cyclopropenyl cation (Cyclic, Planar)	1 π bond	0	1 + 0 + 1 = 2 (even no)	Aromatic
Cyclopropenyl anion (Cyclic, Planar)	1 π bond	1 (For one negative charge on carbon which undergoes delocalization)	1 + 1 + 1 = 3 (odd no)	Anti-aromatic
Cyclobutadiene or [4] annulene (Cyclic, Planar)	2 π bonds	0	2 + 0 + 1 = 3 (odd no)	Anti aromatic
Cyclopentadiene (Cyclic, non planar due to one sp^3 hybridised carbon atom)	2 π bonds	0	2 + 0 + 1 = 3 (odd no)	Non-aromatic
Cyclopentadienyl cation (Cyclic, Planar)	2 π bonds	0	2 + 0 + 1 = 3 (odd no)	Anti-aromatic
Cyclopentadienyl anion (Cyclic, Planar)	2 π bonds	0 (For one negative charge on carbon which undergo delocalization)	2 + 1 + 1 = 4 (even no)	Aromatic
Cyclooctatetraene or [8] annulene (Cyclic, Planar)	4 π bonds	0	4 + 0 + 1 = 5 (odd no)	Anti-aromatic
Cyclooctatrienyl cation (Cyclic, non-planar due to one sp^3 hybridized carbon atom adjacent to positive charge)	3 π bonds	0	3 + 0 + 1 = 4 (even no)	Non aromatic
Pyridine (Cyclic, Planar)	3 π bonds	0 (Here lone pair on N does not take part in delocalization)	3 + 0 + 1 = 4 (even no)	Aromatic
Pyrrole	2 π bonds	1 (Here lone pair on N take part in delocalization)	2 + 1 + 1 = 4 (even no)	Aromatic
Furan	2 π bonds	1 (Here out of two lone pairs on O only one LP take part in delocalization)	2 + 1 + 1 = 4 (even no)	Aromatic
Thiophene	2 π bonds	1 (Here out of two lone pairs on S only one LP take part in delocalization)	2 + 1 + 1 = 4 (even no)	Aromatic

There are some compounds which do not follow the above rule. Huckel's also cannot explain the aromatic or non aromatic behavior of these compounds. These compounds are represented in the Table 2.

Table 2. (Omission behavior of aromatic and non aromatic organic compounds)

Organic Compound (Cyclic, Planar/Cyclic, non-planar)	πb value [πb = number of π bonds with in the ring system]	e^-p value [e^-p = number of delocalized electron pair outside or adjacent to the ring system]	A value [$A = \pi b + e^-p +$ $1(\text{constant})$]	Nature of compound	πb value [πb = number of π bonds with in the ring system]
	5 π bonds	0	5 + 0 + 1 = 6 (even no.)	Not aromatic	Due to the interaction of the hydrogen of 1 and 6 compound become non planar.
	8 π bonds	0	8 + 0 + 1 = 9 (odd no.)	Aromatic	Because double bonded $C_{15}-C_{16}$ do not take part in resonance.

If we easily predict the nature of organic compound i.e. aromatic, anti aromatic or non aromatic then we can resolve different kind of problems regarding stability, reactivity, acidity etc. by using the following supposition.

1) Order of stability is aromatic > non aromatic > anti aromatic

2. Order of reactivity just follows the reverse order of stability as follows:

Anti-aromatic > non aromatic > aromatic

3. Acidity: Stability of Conjugate base α acidity

Eg: cyclopentadienyl anion(aromatic) > cyclopentadiene (non-aromatic) > cyclopentadienyl cation (anti aromatic). Hence, cyclopentadiene (its conjugate base i.e. Cyclopentadienyl anion is aromatic in nature) is much more acidic than cycloheptatriene (its conjugate base i.e. Cycloheptatrienyl anion is anti-aromatic in nature).

3. Conclusions

In conclusion here we approach a new innovative method for easy identification of aromatic, non aromatic and anti aromatic behavior of organic compounds with in very short time. This new method is very helpful to Undergraduate, Graduate and also in Postgraduate level students of chemistry. By using these methods we can easily predict nature of organic compounds in a very simple way.

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