Innovative Mnemonics in Chemical Education

A Handbook for Classroom Lectures

ARIJIT DAS

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By

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PREFACE

The word ‘mnemonic' is derived from the Ancient Greek language. Here, the first letter 'm', in mnemonic is silent. Mnemonics are a memory device, which helps something to be remembered for a long time in the human memory. We remember different colors of the spectrum by ‘VIBGYOR', so, ‘VIBGYOR' acts as a useful mnemonic to remember the colors of the spectrum.

Here, the book entitled, ‘Innovative Mnemonics in Chemical Education’, provides innovative learning techniques in chemical education, which allow students and educators to keep chemical formula for a long time in their memory.

Simple thinking outside the book transports innovation and builds mnemonics and such innovative mnemonics makes chemical education metabolic and intriguing for students and educators both.

In this book, formulae based innovative mnemonics have been discussed to create interest and solve problems of students in the field of organic and inorganic chemical education. Educators can use these mnemonics in their teaching style in the classroom lectures after discussing conventional methods to make chemistry intriguing. Mnemonics allow you to become a successful educator. Here, I have tried to focus some time economic mnemonics by including invented formulae in the field of chemical education. It will encourage students to solve multiple choice type questions (MCQs) in different competitive examinations (NET, NEET, JEE MAIN, JEE ADVANCE, STGT, STPGT etc.) in a time economic way. This book emphasizes chemical education in the light of a variety of mnemonic techniques to make it metabolic, time economic and intriguing for students because the use of mnemonics in classroom lectures is an essential tool to become a distinguished educator.

These mnemonics based innovative methodologies are also suitable for computer-based learning (CBL) activities or for writing computer programs for solving chemistry problems.

It may be expected that this book and its time economic innovative mnemonics would go a long way to help to the students of chemistry at Undergraduate, Senior Undergraduate and Post-Graduate level who would choose the subject as their career. *In vitro* experiments on 100 students showed that by using these formulae students can save up to 30-40 minutes' time in the examination hall. On the basis of this, I can strongly recommend using this book in the field of chemical education.

I would be grateful to the SERB, DST, New Delhi, Govt. of India, for their financial assistance (Sanction no – SERB/F/5537/2013-14 dated 27/11/2013 and D.O. No. SB/EMEQ-014/2013) to carry out my innovative research in the field of Chemical Education.

I would be grateful to the Ministry of Commerce & Industry, Department of Industrial Policy Promotion, Copyright office, Govt. of India, New Delhi for giving me copyright registration certificate bearing registration number L-77140/2018 dated 07/08/2018.

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I want to dedicate this book 'Innovative Mnemonics in Chemical Education (A Handbook for Classroom Lectures)' to my beloved father Late Anil Ranjan Das, who was also a chemistry teacher and was the founder of my chemistry world.

CHAPTER 1

INNOVATIVE MNEMONICS FOR THE PREDICTION OF THE HYBRIDIZATION STATE OF SIMPLE MOLECULES & IONS

In this innovative chapter, formula-based nmemonics count the total number of σ bonds and lone pairs of electrons (T_{SLP}) and then subtract 1 to predict the power of the hybridization state. This method is both innovative and time efficient; it will also enhance the interest of those students who belong to the "paranoia zone of chemistry". Educators can use these nmemonics, after discussing conventional methods, to make chemistry intriguing. This chapter encourages students to solve multiple choice type questions (MCQs) in a time efficient manner to predict the hybridization state of simple molecules and ions; this enables them to find out their normal and sub-normal geometry. This innovative chapter uses a variety of nmemonic techniques to make chemistry fascinating. Also, the use of mnemonics is an essential tool that can be used in classroom lectures.

The conventional formula to determine the hybridization state of simple molecules and ions is time-consuming.[1] Therefore, in this innovative

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[1] L. Pauling, "The Nature Chemical Bond. Application of Results Obtained from the Quantum Mechanics and from a Theory of Paramagnetic Susceptibility to the Structure of Molecules", *J.Am.Chem.Soc.*53(1931):1367 1400, doi:10.1021/ja01355a027, https://pubs.acs.org/doi/abs/10.1021%2Fja01355a027; L. Pauling and P. Pauling, *Chemistry* (Freeman International Ed.: 1975), 148, 163 167; James S. Wright, "Theoretical Evidence for a Stable form of Cyclic Ozone, and its Chemical Consequences", *Can. J. Chem.* 51 (1973): 139 146, http://www.nrcresearchpress.com/doi/10.1139/v73-020#.XEsGBtIza1s; J. D. Lee, *Concise Inorg. Chem.* (Wiley India and Oxford, 5th ed.: 2009), 944, 109 112; J. E. Huheey, et al. *Inorganic Chemistry* (Pearson, 4th ed., India: 2006), 172 185; B. Douglas et al. *Concepts and Models of Inorg. Chem.* (*Wiley India,* 3rd ed.: 2007), 157, 38; F A. Cotton et al. *Basic Inorg. Chem.* (Wiley India, 3rd ed.: 2007), 107, 523, 111.

pedagogical chapter, I have introduced some mnemonics to make chemistry interesting.[2] I have discussed them along with their limitations, applications, and problems.

METHODOLOGY

A. Hybridization state theory

Prof. Linus Pauling (1931), first developed hybridization state theory in order to explain the structure of molecules, such as methane (CH_4), using atomic orbitals. This concept was developed for simple chemical systems but it was applied more widely later on. It is an essential part of finding structures from organic and inorganic compounds.

In hybridization, orbitals from the same atom intermix with slightly different energies and this results in the formation of new orbitals. There are called hybrid orbitals and they have the same energy and shape. The mixing pattern is as follows:

one s + one p = sp hybrid orbital, one s + two p = sp^2 hybrid orbital, one s + three p = sp^3 hybrid orbital, one s + three p + one d (d_{z^2}) = sp^3d hybrid orbital, one s + three p + two d (d_{x2-y2}, d_{z^2}) = sp^3d^2 hybrid orbital, and one s + three p + three d (d_{xy}, d_{yz}, d_{xz}) = sp^3d^3 hybrid orbital.

The ability of the hybrid orbitals to overlap follows the order $sp^3 > sp^2 > sp$. As the p character increases, then it will have more ability to overlap; it will also develop a stronger bond. The bond angles formed by different

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[2] A. Das et.al "Innovative and Time Economic Pedagogical Views In Chemical Education: A Review Article", *World Journal of Chemical Education* 2 (July 2014): 29-38, doi:10.12691/wjce-2-3-1, http://pubs.sciepub.com/wjce/2/3/1/index.html#; A. Das and B. Paul "Time Economic Innovative Pedagogies In Chemical Science: A Review Article", *Education in Chemical Science and Technology, Indian Chemical Society* 3 (Aug 2015): 1 28; A. Das, "A Review of Time Economic Innovative Mnemonics In Chemical Education", *International Journal of Physics and Chemistry Education* 10 (June 2018): 27 40,doi: 10.12973/ijpce/81589: http://www.ijpce.org/A-Review-of-Time-Economic-Innovative-Mnemonics-in-Chemical-Education,81589,0,2.html.

hybrid orbitals are in the order sp (180°) > sp^2(120°) > sp^3(109.5°). A larger s-character creates a greater bond angle. The carbon electronegativity also depends upon the state of hybridization. A larger s-character in hybridization will increase the electronegativity. The order of electronegativity of a C atom is $C_{sp} > C_{sp2} > C_{sp3}$.

Some important facts about hybridization are as follows:

i) Orbitals of comparable energies belonging to same atom or ion can undergo hybridization.
ii) The number of hybrid orbitals is equal to the number of atomic orbitals mixed during hybridization.
iii) Half filled, fully filled, or even empty atomic orbitals with a similar energy can participate in hybridization.
iv) Al hybrid orbitals resulting from a particular type of hybridization will be similar in all respects (same energy, shape, and size).
v) Hybrid orbitals are distributed in space as far apart as possible; therefore, they assign a particular shape and geometry to the molecule.
vi) Hybrid orbitals follow Hund's rule and also Pauli's exclusion principle, just like atomic orbitals.
vii) The bond formed between hybrid orbitals is known as a hybrid bond and this is stronger than non-hybrid bonds of comparable length.
viii) Hybrid orbitals are the "dumb-bell" type with a larger lobe with a +ve sign and a smaller lobe with a -ve sign.

B. The conventional method to predict the hybridization state: VALANCE SHELL ELECTRON PAIR REPULSION THEORY (VSEPR THEORY)

Sidgwick and Powell created VSEPR theory in 1940 and it was further improved by Nyholm and Gillespie in 1957. In a molecule, the central atom is surrounded by shared pairs of electrons (bond pairs), as well as non-bonding electrons (lone pairs). The main concept is that the electron pairs surrounding the central atom repel each other until they no longer react and the molecule is in a state of minimum energy and maximum stability. This arrangement gives a particular shape to the molecules. The order of repulsion between the electron pairs is lone pair–lone pair (LP–LP) > lone pair–bond-pair (LP–BP) > bond pair–bond-pair (BP–BP).

If only bond pairs surround the central atom, the interactions will be equivalent and the molecule will have a regular geometry. If only bond pairs of dissimilar atoms surround the central atom, the interactions will not be equivalent and the molecule will not have a regular geometry. If both bond pairs and lone pairs surround the central atom, the interactions will be very different and the molecular geometry will be distorted.

The conventional formula to predict the hybridization state is $1/2\ (V+MA-C+A)$, where V = number of valance electrons in the central atom, MA = number of surrounding monovalent atoms, C = cationic charge, and A = anionic charge. For example, methane CH_4, $P = 1/2\ (4 + 4 - 0) = 4$ (sp^3 hybridization state); ethylene ($CH_2 = CH_2$), $P = 1/2\ (4 + 2 - 0) = 3$ (sp^2 hybridization state).

C. Innovative mnemonics to predict the hybridization state of simple molecules and ions

i) To predict the sp, sp^2, or sp^3 hybridization state:

Hybridization means mixing orbitals in various ratios; these are called hybrid orbitals. The mixing pattern is s + p (1:1) - sp hybrid orbital; s + p (1:2) - sp^2 hybrid orbital; s + p (1:3) - sp^3 hybrid orbital.

The formula to predict the sp, sp^2, and sp^3 hybridization state is $(P_{Hyb}) = (T_{SLP}) - 1$

Where, P_{Hyb} = power of the hybridization state of the central atom, T_{SLP} = (total no. of σ bonds around each central atom + LP).

From the Lewis structure of a molecule, first predict the number of sigma bonds (σ-bonds), pi bonds (π-bonds), and the lone pair of electrons (LP). All single (-) bonds are σ bonds; in a double bond (=), there is 1σ and 1π; in a triple bond (≡), there is 1σ and 2π (exclude the π bond). In addition to this, each co-ordinate bond (→) can be treated as an σ bond. This formula is applicable up to 4 T_{SLP}. If the power of the hybridization state (P_{Hyb}) is 3, 2, or 1, then the hybridization state will be sp^3, sp^2, and sp, respectively.

ii) In an sp^3d, sp^3d^2, and sp^3d^3 hybridization state, there is a common sp^3 and 4 T_{SLP}. So, for each additional T_{SLP} (an additional sigma bond or lone pair of electrons), add one d orbital gradually as follows:

5 T_{SLP} = 4 T_{SLP} + 1 additional T_{SLP} = sp^3d hybridization
6 T_{SLP} = 4 T_{SLP} + 2 additional T_{SLP} = sp^3d^2 hybridization

$$7\ T_{SLP} = 4\ T_{SLP} + 3 \text{ additional } T_{SLP} = sp^3d^3 \text{ hybridization}$$

In the case of a cationic species, these electrons should be removed from the outermost orbit of the central atom and, in case of an anionic species, remove the outermost electrons of the central atom.[3]

RESULTS AND DISCUSSION

1. Innovative nmemonics to predict the hybridization state of simple molecules and ions

i) Here are some examples that predict the hybridization state (sp, sp^2, and sp^3) of simple molecules and ions:

Example A: NH_3: The central atom N is surrounded by three N-H single bonds (3 sigma σ bonds and an LP). $T_{SLP} = 4$ and, therefore, the power of the hybridization state of N in NH_3 is $(P_{Hyb}) = (T_{SLP}) - 1 = (3+1)-1 = 3$: i.e., the hybridization state = sp^3.

Example B: H_2O: The central atom O is surrounded by two O-H single bonds: i.e., 2 sigma σ bonds and 2 lone pairs. The power of the hybridization state of O is $(P_{Hyb}) = (T_{SLP}) - 1 = = (2+2)-1 = 3$: i.e., the hybridization state of O in $H_2O = sp^3$.

Example C: H_3BO_3: B (Fig. 1.1) only has 3 σ bonds (LP = 0) and oxygen has 2 σ bonds and 2 lone pair of electrons, so, in this case, the power of the hybridization state is $(P_{Hyb}) = (T_{SLP}) - 1 = (3+0)- 1 = 2$: i.e., B is sp^2 hybridized in H_3BO_3. However, the power of the hybridization state is $(P_{Hyb}) = (T_{SLP}) - 1 = = (2+2)-1 = 3$: i.e., the hybridization state of O in H_3BO_3 is sp^3.

Example D: I-Cl: I and Cl both have 1 σ bond and 3 lone pairs of electrons. The power of the hybridization state of both I and Cl, $(P_{Hyb}) = (T_{SLP}) - 1 = (1+3) - 1 = 3$: i.e., the hybridization state of I and Cl is sp^3.

Example E: $CH_2 = CH_2$: Each carbon (Fig. 1.1) is attached with 2 C-H single bonds (2 σ bonds) and 1 C=C bond (1σ bond) and altogether there

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[3] A. Das, "Innovative Mnemonics in Chemical Education: Review Article", *African Journal of Chemical Education* 8, (July 2018): 144 189, https://www.ajol.info/index.php/ajce/article/view/176086; A. Das, "Innovative Mnemonics Make Chemical Education Time Economic: A Pedagogical Review Article", *World Journal of Chemical Education*, 6.4 (Sept 2018): 154 174, doi:10.12691/wjce-6-4-2, http://pubs.sciepub.com/wjce/6/4/2/index.html.

are 3 sigma bonds. The power of the hybridization state of both is C (P_{Hyb}) = (T_{SLP}) – 1= (3+0)-1 = 2: i.e. hybridization state of both carbons is sp^2.

Example F: O_3: Ozone (O_3) exists as a stable form of cyclic ozone (Fig. 1.2) and it is in the shape of an equilateral triangle. Each central O atom has 2 O–O single bonds (2 σ bonds) and 2 LPs. The power of the hybridization state of the central O atom is (P_{Hyb}) = (T_{SLP}) – 1= (2+2) - 1 = 3: i.e., the hybridization state of center atom O in cyclic O_3 is sp^3. However, the resonance description of ozone involves 2 structures (Fig. 1.3), where the central oxygen atom will have an sp^2 hybridization state. In this case, the central O atom has 2 σ bonds and 1 LP. The power of the hybridization state of the central O atom is (P_{Hyb}) = (T_{SLP}) – 1= (2+1) - 1 = 2 (sp^2).

Example G: S_8: The ordinary form of sulfur (orthorhombic sulfur, yellow crystals) contains octatomic molecules (S_8), where S can form single covalent bonds in a long chain with 2 other S atoms in a zigzag fashion (Fig. 1.4). Each sulfur atom is attached with 2 adjacent σ bonds and 2 LPs. The power of the hybridization state of any S atom is (P_{Hyb}) = (T_{SLP}) – 1= (2+2) - 1 = 3: i.e. the hybridization state of S atoms in S_8 is sp^3.

Example H: P_4: The 4 P atoms are arranged at the corners of a regular tetrahedron (Fig. 1.4). Each P atom forms 3 σ bonds and 1 LP. The power of the hybridization state of any P atom is (P_{Hyb}) = (T_{SLP}) – 1= (3+1) - 1 = 3: i.e., the hybridization state of the P atom in P_4 is sp^3.

Example I: CO_3^{2-}: In the valence bond structure of carbonate ion (CO_3^{2-}), the central carbon atom does not contain any lone pair electrons but it does have 3 σ bonds (Fig. 1.5). The power of the hybridization state of the central C atom in carbonate ion is (P_{Hyb}) = (T_{SLP}) – 1= (3+0) - 1 = 2 (sp^2). However, in the resonance hybrid of CO_3^{2-} (Fig. 1.6), the carbon atoms are in a sp^2 hybridization state due to 3 σ bonds and the fact there are no lone pairs of electrons.

ii) Predicting the hybridization state (sp^3d, sp^3d^2, and sp^3d^3) of simple molecules and ions

Example A: I_3^-: The central I atom has 2 σ bonds and 3 lone pairs of electrons (Fig. 1.7). There are 5 T_{SLP}: 5 T_{SLP} = 4 T_{SLP} + 1 additional T_{SLP} = sp^3d hybridization.

Example B: IF_4^+: (Fig. 1.8) There are 7 e^-s in its outermost shell, so subtract one e^- from 7: i.e., 7 – 1 = 6. Out of 6 electrons, 4 electrons form 4

I–F σ bonds and there is 1 LP. Altogether there are 5 T_{SLP}. So, 5 T_{SLP} = 4 T_{SLP} + 1 additional T_{SLP} = sp^3d hybridization.

Example C: XeF_4: (Fig. 1.8) Xe is an inert gas that has 8 e^-s in its outermost shell, 4 form 4 Xe-F sigma bonds and there are 2 lone pair of electrons. Altogether there are 06 T_{SLP} = 4 T_{SLP} + 2 additional T_{SLP} = sp^3d^2 hybridization.

Example D: IF_7: There are 7 I–F single bonds: i.e., 7σ bonds and LP=0. Altogether there are 07 T_{SLP} = 4 T_{SLP} + 3 additional T_{SLP} = sp^3d^3 hybridization.

THE GEOMETRY OF SIMPLE MOLECULES AND IONS

In the absence of lone pair electrons (LPs), a molecule or ion exhibits a regular geometry (Fig. 1.9). For sp, sp^2, sp^3, sp^3d, sp^3d^2, and sp^3d^3 hybridization states, the geometry will be linear, trigonal planar, tetrahedral, trigonal bipyramid, octahedral, and pentagonal bipyramid, respectively. However, for the same hybridization state, and in the presence of the lone pair of electrons, they will exhibit sub-normal geometry (Fig. 1.10). Adequate examples that predict the hybridization state from the corresponding T_{SLP} value (total number of σ bonds around the central atom + lone pair of electrons on the central atom) of the central atom have been explored in Table 1.1. The molecular geometry (normal and sub-normal) and bond angle with respect to the corresponding hybridization state and lone pair of electrons from simple molecules and ions have been displayed in Table 1.2.

THE BOND ANGLE OF SIMPLE MOLECULES AND IONS

The angle between the two covalent bonds of a molecule is called a bond angle. In covalent bonds, the bond pair electron clouds will be adjacent to each other and, due to the excessive force between them, the bond angle will increase. When the bond pair electron clouds move towards the central atom instead of the peripheral atom, then they will be adjacent to each other and exhibit much more repulsive force, which increases the bond angle of the molecule. This is known as a bond pair–bond-pair (BP–BP) repulsion. If there is any other repulsive force greater than this, such as lone pair–lone pair (LP–LP) or lone pair–bond pair (LP–BP) repulsion, the bond angle will decrease. The order of repulsive force is LP–LP > LP–BP > BP–BP.

Factors affecting the bond angle of simple molecules or ions are as follows:

i) Different repulsive force: The order of the bond angle depends on different repulsive forces:

BP–BP > LP–BP > LP–LP.

(LP = 0) (LP = 1) (LP=2)

Therefore, with an increasing number of lone pair electrons, the bond angle will decrease.

Example: The bond angle of methane (CH_4), ammonia (NH_3), and water (H_2O), follows the order: methane (CH_4) > ammonia (NH_3) > water (H_2O). In methane (CH_4), the LP on C = 0 and has a BP–BP repulsion; in ammonia (NH_3), LP of N = 1 and has both LP–BP and BP–BP forces; and in water (H_2O), LP on O = 2 and LP–LP, LP–BP, and BP–BP are all present.

ii) Electronegativity of the central atom (when repulsive force and peripheral atoms are equal): When there are a pair of molecules with an equal repulsive force, the same peripheral atoms but different central atoms, then the bond angle will increase with the electronegativity values due to the greater repulsive interactions between the 2 adjacent bond pair electron clouds.

Example: H_2O and H_2S both exhibit the same repulsive forces (LP–LP, LP–BP, and BP–BP). Here, the peripheral atoms are the same (H) but the central atoms are different (O and S). In oxygen and sulfur, the O central atom in H_2O is more electronegative (E.N. of O = 3.5) than the S central atom in H_2S (E.N. of S = 2.5); therefore, oxygen attracts bond pair electron clouds more closely than sulfur. As a result of this, BP–BP repulsion between two bond pair electron clouds will be greater in H_2O than H_2S.

iii) The electronegativity of the peripheral atom (when the repulsive force and central atoms are the same): When a pair of molecules have the same repulsive force and central atoms but different peripheral atoms the bond angle decreases with the increasing electronegativity values of the peripheral atom. This is due to fewer repulsive interactions between the 2 bond pair electron clouds, which will have been shifted towards the higher electronegative peripheral atom.

Example: NH_3 and NF_3 both have LP =1 and exhibit the same repulsive forces (LP–BP and BP–BP). Here, the central atoms are the same (N) but the peripheral atoms are different (H and F). The peripheral atom (F) in NF_3 is more electronegative (E.N. of F = 4.0) than the peripheral atom (H) in NH_3 (E.N. of H = 2.1). Fluorine attracts bond pair electron clouds more closely than hydrogen. As a result of this, BP–BP repulsion between the 2 adjacent bond pair electron clouds will be greater in NH_3 than NF_3.

APPLICATIONS FOR THE HYBRIDIZATION STATE:

1. The hybridization state used to predict the dipole moment (μ) as well as polarity.

Example A: Cis-2-butene is polar, while trans-2-butene is a non-polar (Fig. 1.11). The % of s character is directly proportional to electronegativity; therefore, the order of electronegativity is sp - C (s 50%) > sp^2 - C (s 33.3%) > sp^3 - C (s 25%)

2. The hybridization state used to predict the acidic order of hydrocarbons (alkyne, alkene, and alkane).

Example B: The acidic order of alkyne, alkene, and alkane is sp sp, sp^2 sp^2, and sp^3 sp^3

The decreasing acidic order is alkyne ($HC \equiv CH$) > alkene ($H_2C = CH_2$) > alkane ($H_3C - CH_3$)

Alkyne has sp hybridized carbon atoms, alkene has sp^2 hybridized carbon atoms, and alkane has sp^3 hybridized carbon atoms: % of s character $\propto$ electronegativity and electronegativity of carbon in hydrocarbons $\propto$ proton donation tendency (acidity). The electronegativity order is sp - C (s 50%) > sp^2 - C (s 33.3%) > sp^3 - C (s 25%) and the decreasing acidic order is alkyne ($HC \equiv CH$) > alkene ($H_2C = CH_2$) > alkane ($H_3C - CH_3$).

3. The hybridization state used to predict the basic order.

Example C: Basic strength between amine ($-NH_2$) and nitrile ($-CN$) can be explained as follows:

Nitrogen atom in methylamine (CH_3NH_2) is sp^3 hybridized (% s character = 25%) and in methyl cyanide ($CH_3C{\equiv}N$) is sp hybridized (% s character = 50%). With % s character, the electronegativity increases. Hence, sp N of methyl cyanide ($CH_3C{\equiv}N$) is more electronegative than methylamine (CH_3NH_2), which (sp N of methyl cyanide) tightly holds the lone pair of electrons and is less readily available for protonation or donation. This decreases the basic character of methyl cyanide ($CH_3C{\equiv}N$) with respect to methylamine (CH_3NH_2).

4. The hybridization state used to predict normal and sub-normal geometry.

Simple molecules or ions with LP = 0 have a normal geometry, while LP ≠ 0 have sub-normal geometry (Table 1.2).

5. The hybridization state used to predict the bond length and strength.

The power of the hybridization state (P_{Hyb}) is directly proportional to bond length and inversely proportional to the bond strength. Generally, mixing the hybridization state decreases the bond length.

Example D:

C-C: sp^3-sp^3, $P_{Hyb} = 3+3 = 6$, C-C bond length = 1.54Å

C-C sp^3-sp^2, $P_{Hyb} = 3+2 = 5$, C-C bond length = 1.50Å

C-C: sp^3-sp, $P_{Hyb} = 3+1 = 4$, C-C bond length = 1.46Å

C=C: sp^2-sp^2, $P_{Hyb} = 2+2 = 4$, C-C bond length = 1.34Å

C=C sp^2-sp, $P_{Hyb} = 2+1 = 3$, C-C bond length = 1.31Å

C≡C: sp-sp, $P_{Hyb} = 1+1 = 2$, C-C bond length = 1.21Å

C-H: sp^3-H, $P_{Hyb} = 3$, C-H bond length = 1.11Å

sp^2-H, $P_{Hyb} = 2$, C-H bond length = 1.10Å

sp-H, $P_{Hyb} = 1$, C-H bond length = 1.08Å

C-O: sp^3-O, $P_{Hyb} = 3$, bond length = 1.41Å

C=O: sp^2-O, $P_{Hyb} = 2$, bond length = 1.20Å

C-N: sp^3-N, $P_{Hyb} = 3$, bond length = 1.47Å

C=N: sp^2-O, $P_{Hyb} = 2$, bond length = 1.28Å

C≡N: sp-N, $P_{Hyb} = 1$, bond length = 1.16Å

6. The bond angle can also be evaluated from the hybridization state.

The bond angle is directly proportional to the s character of a hybrid orbital: $sp - C$ (50 % s) > $sp^2 - C$ (33.3 % s) > $sp^3 - C$ (25% s)

QUESTIONS ON HYBRIDIZATION AND GEOMETRY

Q1. Which of the following pairs of ions is isoelectronic and isostructural? (NEET II-2016)

a) CO_3^{2-}, NO_3^- b) ClO_3^-, CO_3^{2-} c) SO_3^{2-}, NO_3^- d) ClO_3^-, SO_3^{2-}

Ans: both (a) and (d) (CO_3^{2-}, NO_3^- both have 32 e^-s, sp^2, LP=0, trigonal planar geometry) and (ClO_3^-, SO_3^{2-} both have 42 e^-s, sp^3, LP=1, pyramidal geometry)

Q2. The correct geometry and hybridization for XeF_4 are (NEET II 2016)

a) octahedral, sp^3d^2 b) trigonal bipyramidal, sp^3d c) planar triangle, sp^3d^3 d) square planar, sp^3d^2

Ans: (d) square planar, sp^3d^2

Q3. XeF_2 is iso-structural with (NEET 2013)

a) $SbCl_3$ b) $BaCl_2$ c) TeF_2 d) ICl_2^-

Ans: (d) ICl_2^- sp^3d linear

Q4. The strucure of IF_7 is (AIEEE 2011)

a) square pyramid b) trigonal bipyramid c) octahedral d) petagonal bipyramid

Ans: (d) IF_7 - sp^3d^3 LP=0, petagonal bipyramid (normal geometry).

Q5. Consider the state of hybridization in carbon atoms and find the linear the molecule (CBSE PMT 2011)

a) $CH_3 - CH = CH - CH_3$ b) $CH_3 - C \equiv C - CH_3$

c) $CH_2 = CH - CH_2 - C \equiv CH$ d) $CH_3 - CH_2 - CH_2 - CH_3$

Ans: (b) $CH_3 - C \equiv C - CH_3$ (both $- C \equiv C -$ will be in a sp hybridization state and LP = 0)

Q6. Base strength of $H_3C\text{-}CH_2^-$ (i), $H_2C = CH^-$ (ii) and $H - C \equiv C^-$ (iii) is in which order?

a) (i) > (iii) > (ii) b) (i) > (ii) > (iii) c) (ii) > (i) > (iii) d) (iii) > (ii) > (i)

Ans: (b) (i) > (ii) > (iii), acidic order is $H\text{-}C \equiv C\text{-}H > H_2C = CH_2 > H_3C\text{-}CH_3$ as a stronger acid will have a weaker conjugate base; therefore, the order is $H_3CCH_2^- > H_2C = CH^- > H - C \equiv C^-$.

Q7. Methylamine (CH_3NH_2) is more basic than methyl cyanide ($CH_3C{\equiv}N$). Why?

a) both have a different (+I) group b) both have the same (+I) group

c) both nitrogens have the same s character d) both nitrogens have a different s character

Ans: (d) both nitrogens have a different s character

Q8. Which of the following species contains 3 bond pairs and one LP around the central atom? (NEET 2013)

a) H_2O b) BF_3 c) NH_2^- d) PCl_3

Ans: (d) PCl_3 (LP = 1 and BPs = 3)

Q9. What is the hybridization of atomic orbitals in NO_2^+, NO_3^-, and NH_4^+? (NEET 16) (JEE MAIN 16)

a) sp, sp^3 and sp^2 b) sp^2, sp^3 and sp c) sp, sp^2, and sp^3 d) sp^2, sp, and sp^3

Ans: (c) sp, sp^2, and sp^3

Q10. The total number of lone pair electrons in I_3^- ion is (JEE MAIN 2018)

a) 3 b) 6 c) 9 d) 12

Ans: (c) 9

Q11.Which of the following molecules represents the order of hybridization (sp^2, sp^2, sp) from left to right (NEET18)

a) $CH_2=CH-CH=CH_2$ b) $CH_2=CH-C\equiv CH$ c) $CH\equiv C-C\equiv CH$ d) $CH_3-CH=C=CH_2$

Ans: (b) $CH_2=CH-C\equiv CH$ (This demonstrates the limitations of the conventional method)

Q12. Which of the following pair have sp^3 hybridization? (Karnataka NEET 2013)

a) SiF_4, BeH_2 b) NF_3, H_2O c) NF_3, BF_3 d) H_2S, BF_3

Ans: (b) NF_3, H_2O

Q13. The correct geometry and hybridization for XeF_4 are (NEET II 2016)

a) octahedral, sp^3d^2 b) trigonal bipyramidal, sp^3d c) planar triangle, sp^3d^3 d) square planar, sp^3d^2

Ans: (d) square planar, sp^3d^2

Q14. Which of the following bonds is the strongest?

a) H_3C-CH_3 b) $H_2C=CH_2$ c) $H_3C-CH=CH_2$ d) $HC\equiv CH$

Ans: (d) $HC\equiv CH$

Q15. Which of the following is planar?

a) methane b) acetylene c) benzene d) isobutane

Ans: (c) benzene (all six carbons are sp^2 hybridized, which makes it planar)

Q16. The order of bond length of C–C in ethane (I), ethene (II) and ethyne (III) is

a) I > II > III b) II > I > III c) III > I > II d) III > II > I

Ans: (a) I > II > III (I (ethane, sp^3, $P_{Hyb}=3$) > II (ethene, sp^2, $P_{Hyb}=2$) > III (ethyne, sp, $P_{Hyb}=1$))

Q.17. Which of the following carbon atoms is most electronegative?

a) I b) II c) III d) all are equally electronegative

Ans: (a) (sp C, s 50 %, % of s character ∝ electronegativity)

Q.18. An sp^3 hybrid orbital contains

a) 1/4 s-character b)1/2 s-character c) 2/3 s-character d) 3/2 s-character

Ans: (a) 1/4 s-character (s:p = 1:3 in sp^3)

Q.19. In CCl_4, the four valences of carbon are directed towards the corner of a

a) cube b) hexagon c) prism d) tetrahedron

Ans: (d) tetrahedron (In CCl_4 - C is in sp^3, BP = 0 and LP of C = 0, regular geometry) (See Table 1.2)

Q.20. Which has the largest angle between the two covalent bonds?

a) H_2O b) NH_3 c) CO_2 d) CH_4

Ans: (c) CO_2 (In O=C=O, hybridization sp and bond angle 180°) (See Table 1.2)

Q.21. Which has the smallest bond angle?

a) H_2O b) H_2S c) NH_3 d) CH_4

Ans: (b) H_2S (Bond angle ∝ 1/number of LPs and the repulsive force; bond angle ∝ and electronegativity of the central atom)

Q.22. Which of the following is associated with the compound where the central atom has sp^3d hybridization?

a) planar b) pyramidal c) angular d) trigonal bipyramidal

Ans: (d) trigonal bipyramidal (See Table 1.2)

Q.23. The pyramidal geometry is associated with

a) CH_4 b) NH_3 c) H_2O d) CO_2

Ans: (b) NH_3 (See Table 1.2)

Q.24. According to VSEPR theory, which one of the following has an ideal tetrahedral shape? (NET 2011)

a) SO_2 b) SO_3 c) SO_4^{2-} d) SO_3^{2-}

Ans: (c) SO_4^{2-} (SO_4^{2-} is ideal because of the presence of equal atoms and it has LP = 0 and BP = 4 around the S atom) (See Table 1.2)

Q.25. Which of the following molecules is linear?

a) C_2H_2 b) $SiCl_4$ c) CH_4 d) H_2Se

Ans: (a) C_2H_2 (H-C≡C-H, sp-C, LP= 0, linear geometry)

Q.26. Boron in BCl_3 has (NET 2017)

a) sp hybridization b) sp^2 hybridization c) sp^3 hybridization d) no hybridization

Ans: (b) sp^2 hybridization (See Table 1.1)

Q.27. The molecule where sp^2 hybrid orbitals are used by the central atom to form covalent bonds is known as

a) He_2 b) SO_2 c) PCl_5 d) N_2

Ans: (b) SO_2 (See Table 1.2)

Q.28. The bond angle in NH_3 is close to

a) 90° b) 180° c) 109° d)120°

Ans: (c) 109°

Q.29. The octahedral shape is associated with

a) PF_5 b) SF_4 c)TeF_6 d) ClF_3

Ans: (c) TeF_6 (LP of Te = 0, sp^3d^2 - octahedral) (See Table 1.2)

Q.30. The hybrid states of carbon in diamond, graphite, and acetylene are, respectively

a) sp^2, sp, sp^3 b) sp, sp^2, sp^3 c) sp^3, sp^2, sp d) sp^2, sp^3, sp

Ans: (c) sp^3, sp^2, sp (in diamond C - sp^3, in graphite C - sp^2, and in acetylene C - sp)

Q.31. The AsF_5 molecule is trigonal bipyramidal. The orbitals used by As for hybridization are

a) d_{z^2}, s, p_x, p_y, p_z b) d_{x2-y2}, s, p_x, p_y, p_z c) s, p_x, p_y, p_z, d_{xz} d) none of the above

Ans: (a) d_{z^2}, s, p_x, p_y, p_z (see earlier in this chapter)

Q.32. Using VSEPR theory, the molecule with the highest number of LPs and a linear shape is (NET 2011)

a) CO_2 b) I_3^- c) NO_2 d) NO_2^+

Ans: (b) I_3^- (Tri iodide ion I_3^- has a linear geometry in which the central I contains 3 LPs; see Fig. 1.7)

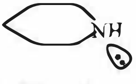
Q.33. Which of the following molecules/ions has a triangular pyramidal shape?

a) BF_3 b) NO_3^- c) H_3O^+ d) CO_3^{2-}

Ans: (c) H_3O^+ (It is sp^3 hybridized with 1 LP and 3 BPs around the oxygen atom. This is similar to NH_3. It also has a triangular pyramidal shape; see Fig. 1.10)

Q.34. In piperidine, the hybrid state assumed by N is

a) sp b) sp^2 c) sp^3 d) dsp^2

Ans: (c) sp^3 

(In piperidine, N is surrounded by 01 LP and 3 BPs – sp^3 hybridized)

Q.35. Which of the following pairs contains the isostructural species?

a) CH_3^- and CH_3^+ b) NH_4^+ and NH_3 c) SO_4^{2-} and BF_4^- d) NH_2^- and BeF_2

Ans: (c) SO_4^{2-} and BF_4^- (both are sp^3 hybridized and have tetrahedral geometry)

Q.36. The BCl_3 molecule is planar, while NCl_3 is pyramidal because

a) BCl_3 does not have the lone pair on B but NCl_3 has one b) the N atom is smaller than B c) the B-Cl bond is more polar than the N-Cl bond d) the N-Cl bond is more covalent than the B-Cl bond

Ans: (a) BCl_3 does not have the lone pair on B but the NCl_3 has one (See Table 1.2)

Q.37. According to VSEPR theory, in SF_4, BF_4^-, XeF_4, and ICl_4^-, the number of species with two LP on the central atom is (NET 2011)

a) 2 b) 3 c) 4 d) 0

Ans: (a) 2 (XeF_4 and ICl_4^- both have LP =2; see Table 1.2)

Q.38. The total number of Xe lone pairs of electrons in $XeOF_4$ is/are

a) 0 b) 1 c) 2 d) 3

Ans: (b) (LP = 1 and BPs = 6 around Xe in $XeOF_4$)

Q.39. The angles between covalent bonds is highest in

a) CH_4 b) BF_3 c) PF_3 d) NH_3

Ans: (b) BF_3 (sp^2 hybridized has the highest bond angle, while the others are sp^3 hybridized with a lower bond angle)

Q.40. The bond length between the C--C bonds in sp^2 hybridized molecule is

a) 1.2Å b) 1.62Å c) 1.54Å d) 1.34Å

Ans: (d) 1.34Å (C=C: sp^2-sp^2, C-C bond length = 1.34Å)

Q.41. The hybridization of Xe in XeF_2 is

a) sp^3 b) sp^2 c) sp^3d d) sp^3d^2

Ans: (c) sp^3d (BPs = 2 and LPs = 3 around Xe in XeF_2 - 5 T_{SLP} = 4 T_{SLP} + 1 additional T_{SLP} = sp^3d hybridization)

Q.42. Which of the following is octahedral?

a) SF_6 b) BF_4^- c)PCl_5 d) H_3BO_3

Ans: (a) SF_6 (LP = 0, sp^3d^2 – regular geometry = octahedral)

Q.43. The structure of CH_2=C=CH_2 is

a) linear b) planar c) non-planar d) none of the above

Ans: (b) Planar (since carbon only uses sp and sp^2 hybrid orbitals)

Q.44. Carbon atoms in benzene molecule are inclined at an angle of

a) 120° b) 180° c) 109° d) 60°

Ans: (a) 120° (in benzene, each carbon atom is sp^2 hybridized)

Q.45. In a BrF_3 molecule, the lone pairs occupy equatorial positions to minimize

a) lone pair–lone pair repulsion only b) lone pair–bond pair repulsion only c) bond pair–bond pair repulsion only d) lone pair–lone pair repulsion and lone pair–bond pair repulsion

Ans: (d) lone pair–lone pair repulsion and lone pair–bond pair repulsion

Q.46. The shape of gaseous $SnCl_2$ is

a) tetrahedral b) linear c) angular d) T-shaped

Ans: (c) angular (Sn is sp^2 hybridized and angular shaped)

Q.47. The shape of the molecule SF_2Cl_2 is

a) trigonal bipyramidal b) cube c) octahedral d) tetrahedral

Ans: (a) trigonal bipyramidal (in SF_2Cl_2, LP=1 and BPs = 4, hence, 5T_{SLP} = 4 T_{SLP} + 1 additional T_{SLP} = sp^3d hybridization)

Q.48. Which carbon is more electronegative?

a) sp^3-hybridized carbon b) sp-hybridized carbon c) sp^2-hybridized carbon d) Irrespective of the hybrid state

Ans: (b) sp-hybridized carbon (% s = 50%)

Q.49.The shape of O_2F_2 is similar to

a) C_2F_2 b) H_2O_2 c) H_2F_2 d) C_2H_2

Ans: (b) H_2O_2

Q.50. The most efficient overlap is

a) sp^2-sp^2 b) s-s c) sp^3-sp^3 d) sp-sp

Ans: (c) sp^3-sp^3 (The larger the p-character, the greater its ability to overlap)

Q.51. In NO_3^- ion, the number of bond pairs and lone pairs of electrons are

a) 2, 2 b) 3, 1 c) 1, 3 d) 5, 8

Ans: (d) 4, 8 (NO_3^- is the conjugate base of HNO_3 where BPs = 5 and LPs of O = 8)

Q.52. The shape of ClO_3^- is

a) triangular pyramidal b) tetrahedral c) angular d) linear

Ans: (b) tetrahedral (In ClO_3^- LP = 0 sp^3 hybridization state)

Q.53. IF_5 has the following hybridization

a) sp^3d^2 b) sp^3d c) sp^3d^3 d) none of the above

Ans: (a) sp^3d^2 (LP = 1 and BPs = 5, hence, 6 T_{SLP} = 4 T_{SLP} + 2 additional T_{SLP} = sp^3d^2 hybridization)

Q.54. The correct order of the bond angle is

a)$H_2O > NH_3 > CH_4 > CO_2$ b) $H_2O < NH_3 < CO_2 < CH_4$ c) $H_2O < NH_3 > CO_2 > CH_4$ d) $CO_2 > CH_4 > NH_3 > H_2O$

Ans: (d) $CO_2 > CH_4 > NH_3 > H_2O$ (In CO_2 LP = 0, linear, sp; in CH_4 LP = 0, tetrahedral, sp^3; in NH_3, LP =1, sp^3 and in H_2O, LP = 2, sp^3)

Q.55. In OF_2, the number of bond pairs and lone pairs of electrons are

a) 2, 6 b) 2, 8 c) 2,10 d) 2, 9

Ans: (b) 2, 8 (In F-O-F, each F has 3 LPs and O has 2 LPs; BPs = 2)

Q.56. Which of the following bonds requires the largest amount of bond energy to dissolve it into corresponding atoms?

a) H-H bond in H_2 b) C-H bond in CH_4 c) N≡N bond in N_2 d) O=O bond in O_2

Ans: (c) N≡N bond in N_2 (BO is directly proportional to the bond dissociation energy; the BO of N_2 is 3.0; the greater the multiplicity of the bond, the greater the bond strength and the bond dissociation energy)

Q.57. A beryllium atom in BeF_2 is

a) sp^3 hybridized b) sp^2 hybridized c) sp hybridized d) unhybridized

Ans: (c) sp hybridized (In BeF_2, Be has LP = 0 and σ bonds = 2, $(P_{Hyb}) = (T_{SLP}) - 1 = 2 - 1 = 1$ (sp))

Q.58. Which molecule is linear?

a) ICl b) NO_2 c) SO_2 d) ClO_2

Ans: (a) ICl (In ICl, the LP of each halogen = 3, σ bond = 1, $(P_{Hyb}) = (T_{SLP}) - 1 = 4 - 1 = 3$ (sp^3), linear)

Q.59. The molecule with the largest distance between the two adjacent carbon atoms is

a) ethane b) ethene c) ethyne d) benzene

Ans: (a) ethane (sp^3; the lower the multiplicity of the bond, the higher the bond length)

Q.60. The correct sequence for the decrease in the bond angles is

a) $NH_3 > PH_3 > AsH_3 > SbH_3$ b) $NH_3 > AsH_3 > PH_3 > SbH_3$ c) $SbH_3 > AsH_3 > PH_3 > NH_3$ d) $PH_3 > NH_3 > AsH_3 > SbH_3$

Ans: (a) $NH_3 > PH_3 > AsH_3 > SbH_3$ (under the same repulsive force, the bond angle is directly proportional to the electronegativity of the central atom; when the peripheral atoms are equal, the electronegativity order is N>P>As>Sb)

Q.61. The compound where C uses its sp^3 hybrid orbitals for bond formation is

a) $HCOOH$ b) $(H_2N)_2CO$ c) $HCHO$ d) CH_3CHO

Ans: (d) CH_3CHO (CH_3 group in CH_3CHO is sp^3 hybridized)

Q.62. The correct order of the increasing C-O bond length is

a) $CO_3^{2-} < CO_2 < CO$ b) $CO_2 < CO_3^{2-} < CO$ c) $CO < CO_3^{2-} < CO_2$ d) $CO < CO_2 < CO_3^{2-}$

Ans: (d) $CO < CO_2 < CO_3^{2-}$ (Resonance is possible in CO_3^{2-}, $O = C = O$, $C \equiv O$)

Q.63. Select the pair where the two species are not isostructural

a) PF_6^- and SF_6 b) SiF_4 and SF_4 c) XeF_2 and BrCl d) BH_4^- and NH_4^+

Ans: (b) SiF_4 and SF_4 (SiF_4, tetrahedral, sp^3 and SF_4, see-saw, sp^3d) (see Table 1.2)

Q.64. The number of σ and π bonds in pent-4-ene-1-yne are

a) 3, 10 b) 9, 4 c) 4, 9 d) 10, 3

Ans: (d) 10,3 ($H\equiv C\text{-}CH_2\text{-}CH=CH_2$, all single bonds are σ bonds, double bonds are 1σ and 1π, triple bonds are 1σ and 2π)

Q.65. A lone pair of electrons is present in the central atom of (STGT 2018)

a) CCl_4 b) BF_3 c) NH_3 d) None of the above

Ans: (c) NH_3 (for N, LP =1, BPs=3)

Q.66. The C-C bond length in ethane molecule is (STGT 2018)

a) 1·20 Å b) 1·54 Å c) 1·34 Å d) 1·39 Å

Ans: (b) 1·54 Å (in ethane, C-C: sp^3-sp^3, $P_{Hyb} = 3+3 = 6$, C-C bond length = 1.54Å)

Q.67. The C-C-C bond angle in diamond crystal is (STGT 2018)

a) 109°28' b) 107°28' c) 120° d) None of the above

Ans: (a) 109°28' (in diamond, C - sp^3 and in graphite C - sp^2)

Q.68. In crystalline graphite, the C-C bond length is (STGT 2017)

a) 1·54 Å b) 1·34 Å c) 1·42 Å d) 1·62 Å

Ans: (b) 1·34 Å (in graphite, C-C: sp^2-sp^2, $P_{Hyb} = 2+2 = 4$, C-C bond length = 1.34 Å)

Q.69. What is the C-C bond length (in angstrom) in diamond? (STGT 2016)

a) 5·2 b) 2·0 c) 1·54 d) 3·35

Ans: (c) 1·54 (in diamond, C-C: sp^3-sp^3, $P_{Hyb} = 3+3 = 6$, C-C bond length = 1.54 Å)

Q.70.The ratio of σ and π bonds in naphthalene is (STGT 2016)

a) 1: 5 b) 5:11 c) 8:5 d) 19:5

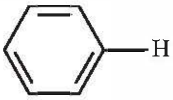
Ans: (d) 19:5 (in naphthalene, there are 19 σ and 5π bonds)

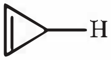
Q.71. Which ClO_3^-, XeO_3, and SO_3 species have a pyramidal shape? (NET 2017)

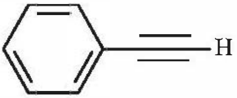
a) ClO_3^- and XeO_3 b) XeO_3 and SO_3 c) ClO_3^- and SO_3 d) SO_3

Ans: (a) ClO_3^- and XeO_3 (see Table 1.2)

Q.72. The correct order of the bond dissociation energy for the indicated C-H bond in the following compounds is (NET 2016)

A) 

B) 

C) 

a) C > B > A b) A > B > C c) A > C > B d) C > A > B

Ans: (d) C > A > B [The power of the hybridization state (P_{Hyb}) of a hydrogen bonded carbon atom is directly proportional to the bond length and bond length is inversely proportional to the bond dissociation energy. In A: sp^2-H, P_{Hyb} = 2, C-H bond length = 1.10Å; in B: sp^3-H, P_{Hyb} = 3, C-H bond length = 1.11Å; and in C sp-H, P_{Hyb} = 1, C-H bond length = 1.08Å.

Q.73. Using VSEPR theory, the correct shape of [TeF$_5$]$^-$ ion is (NET 2016)

a) trigonal bipyramidal b) square pyramidal c) pentagonal planar d) see-saw

Ans: (b) square pyramidal (see Table 1.2)

It can be expected that these 4 time efficient innovative mnemonics will help the students of chemistry at undergraduate, senior undergraduate and postgraduate level. Experiments, *in vitro*, on 100 students, showed that these nmemonics students could save up to 3–5 minutes in the examination hall. On the basis of this, I can strongly recommend using these techniques in chemical education.

CHAPTER 2

INNOVATIVE MNEMONICS FOR THE PREDICTION OF THE HYBRIDIZATION STATE OF ORGANIC COMPOUNDS

In the previous chapter, formulae-based nmemonics counted the total number of σ bonds and the lone pairs of electrons around the central atom and then subtracted 1 from this total value (T_{SLP}) to predict the power of the hybridization state. This was done in an innovative and time efficient way in order to engage students who belong to the "paranoia zone of chemistry". This chapter uses other formulae-based mnemonics, which count total number of σ bonds and localized negative charge (T_{SLNC}) or the localized lone pairs of electrons (T_{SLLP}) and then subtracts 1 from this total value (T_{SLNC} or T_{SLLP}) to predict the power of the hybridization state of carbon atoms and heteroatoms in different organic compounds, including heterocyclic compounds. This has been done in an innovative and time efficient way. Educators can use these mnemonics in their classroom lectures after discussing conventional methods and their limitations to make chemistry intriguing.

I have included 2 formulae to predict the hybridization of carbon atoms and heteroatoms in different organic compounds. This encourages students to solve multiple choice type questions (MCQs) in different competitive examinations in a time efficient manner. Predicting the hybridization state in different organic compounds is also useful with regard to the planarity of compounds, which is essential when evaluating the aromaticity of organic compounds. This chapter uses a variety of mnemonics to make organic chemistry organic, time efficient, and intriguing for students because it is an essential tool that will help you become a distinguished educator. The conventional method to predict the hybridization state of carbon and heteroatoms in organic compounds in order to find out the planarity of compounds is time consuming.[4] I have introduced two innovative mnemonics to make this innovative pedagogical chapter intriguing in all respects.[5]

METHODOLOGY

1. Classifying negative charge inorganic compounds

The negative charge on the carbon atom of any ring system can be generally classified into two types: a delocalized negative charge (DNC) and a localized negative charge (LNC).

a) Delocalized negative charge (DNC): When the negative charge on the carbon atom from a ring system of an organic compound undergoes delocalization through conjugation then it is treated as a DNC. When a negative charge bearing carbon atom is directly attached with single bonds from all ends to the ring system of an organic compound then it is considered to be a DNC containing carbon atom.

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[5] A. Das *et al.*, "A rapid and innovative method for the identification of aromatic and anti-aromatic nature of organic compounds", *World Journal of Chemical Education* 1 (Sept 2013): 6 8, doi: 10.12691/wjce-1-1-2, http://pubs.sciepub.com/wjce/1/1/2/#; A. Das, "Innovative and Time Economic Pedagogical Views In Chemical Education - A Review Article", *World Journal of Chemical Education* 2 (July 2014): 29-38, doi:10.12691/wjce-2-3-1, http://pubs.sciepub.com/wjce/2/3/1/index.html#; A. Das, "Lone Pair Electron Discriminate Hybridization with Aromatic and Anti Aromatic behavior of Heterocyclic Compounds - Innovative Mnemonics", *World Journal of Chemical Education* 6 (April 2018): 95 101, doi: 10.12691/wjce-6-2-4, http://pubs.sciepub.com/wjce/6/2/4/; A. Das, "A Review of Time Economic Innovative Mnemonics In Chemical Education", *International Journal of Physics & Chemistry Education* 10, (June 2018): 27 40, doi: 10.12973/ijpce/81589, http://www.ijpce.org/A-Review-of-Time-Economic-Innovative-Mnemonics-in-Chemical-Education,81589,0,2.html; A. Das, "Innovative Mnemonics In Chemical Education: Review Article", *African Journal of Chemical Education* 8, (July 2018): 144 189, https://www.ajol.info/index.php/ajce/article/view/176086.

Example: In cyclopropenyl anions, cyclopentadienyl anions, and cycloheptatrienyl anions (Fig. 2.12, Fig. 2.13, and Fig. 2.14) the negative charge in the C atom is to be treated as a DNC because it is directly attached with single bonds on all sides.

b) Localized negative charge (LNC): When the negative charge on the carbon atom from the ring system of an organic compound does not undergo delocalization through conjugation then it is to be treated as an LNC. When a negative charge bearing carbon atom from the ring system of an organic compound is directly attached with single and double bonds, it should be treated as an LNC containing carbon atom and with an LNC negative charge.

2. Classifying a lone pair of electrons in heterocyclic compounds

A lone pair of electrons can be generally classified into two types: delocalized lone pair electrons (DLP) and localized lone pair electrons (LLP).

a) Delocalized lone pair electron (DLP): When the lone pair of electrons from a heteroatom undergoes delocalization through conjugation then it is to be treated as a DLP. When a heteroatom is directly attached with single bonds from all ends, it should be considered to be a DLP-based heteroatom and its lone pair should also be treated as such.

Example In Pyrrole (Fig. 2.16), the lone pair of N atom should be treated as a DLP because it is directly attached with only three single bonds.

b) Localized lone pair electron (LLP): When the heteroatom's lone pair of electrons do not undergo delocalization through conjugation then it should be treated as an LLP. When the heteroatom is directly attached to the ring system with single and double bonds then it should be considered as an LLP-based heteroatom and its lone pair should also be treated as such.

Example: In Pyridine (Fig. 2.16), the lone pair of N atom should be treated as an LLP because it is directly attached with double and single bonds to the ring system.

3. Planarity of organic compounds

Knowing the planarity is essential when predicting the aromatic, anti-aromatic, and non-aromatic behavior of heterocyclic or other organic compounds. For aromatic and anti-aromatic behavior, the compound must be planar, while the non-planar compound is non-aromatic in nature. The planarity of heterocyclic compounds depends on the nature of the hybridization state of carbons and the heteroatoms present. When all atoms (carbon and hetero) in the heterocyclic compound are sp^2 hybridized then it is planar, but when there is a mixture of sp^2 and sp^3 hybridization states then it is treated as non-planar

4. The conventional method for predicting the hybridization state of organic compounds

The hybridization state of a molecule can be calculated using $P = 1/2\ (V+MA-C+A)$

Where V = number of valance electrons in the central atom, MA = number of surrounding monovalent atoms, C = cationic charge, A = anionic charge, and P = power of the hybridization state of the central atom.

5. Innovative mnemonics to predict the hybridization state of carbon atom in organic compounds

The formula to predict the sp^2 and sp^3 hybridization state:

Power of the hybridization state of the heteroatom (P_{Hyb}) = (T_{SLNC}) – 1

Where P_{Hyb} = power of the hybridization state of the heteroatom, T_{SLNC} = (total no. of σ bonds around each central atom + LNC), and LNC = localized negative charge.

All single (-) bonds are σ bonds and, in a double bond (=), there is one σ and one π. If the power of the hybridization state (P_{Hyb}) is ●3, ●2, and ●1, then the hybridization state will be sp^3, sp^2, and sp, respectively.

6. Innovative mnemonics to predict the hybridization state of a heteroatom in different heterocyclic compounds

Formula to predict the sp^2 and sp^3 hybridization state:

Power of the hybridization state of the heteroatom (P_{Hyb}) = (T_{SLLP}) – 1, where P_{Hyb} = power of the hybridization state of the heteroatom, T_{SLLP} = (total no. of σ bonds around each central atom + LLP), and LLP = localized lone pair of electrons.

If the power of the hybridization state (P_{Hyb}) is ●3, ●2, and ●1 then the hybridization state will be sp^3, sp^2, and sp, respectively. All single (-) bonds are σ bonds and, in a double bond (=), there is one σ and one π.

RESULTS AND DISCUSSION

1. Innovative mnemonics to predict the hybridization state (sp^2 and sp^3) of carbon atoms in organic compounds

The hybridization state of a carbon atom in organic compounds can be calculated from the total number of σ bonds around the carbon atom and the number of its localized negative charge (T_{SLNC}) on the carbon atom. Subtract 1 from this value of T_{SLNC} to get the hybridization state (sp^2 and sp^3).

Example A: In cyclopropene, cyclopentadiene, and cycloheptatriene (Fig. 2.12, Fig. 2.13, Fig. 2.14), the vertex carbon atom is in an sp^3 hybridization state. In all cases, the vertex carbon atom is surrounded by 4 single bonds (σ bonds) and the power of the hybridization state is (P_{Hyb}) = (T_{SLNC}) – 1 = 4-1 = 3 (sp^3). The rest of the carbon atoms have an sp^2 hybridization state that corresponds to 3σ bonds (2 single bonds and 1 double bond). The presence of 1 sp^3 hybridized carbon atom along with other sp^2 hybridized carbons makes cyclopropene, cyclopentadiene, and cycloheptatriene non-planar.

Example B: In cyclopropenyl anions, cyclopentadienyl anions, and cycloheptatrienyl anions (Fig. 2.12, Fig. 2.13, and Fig. 2.14), the vertex carbon atom that has negative charge is in an sp^2 hybridization state. In all cases, the vertex carbon atom is surrounded by 3 single bonds (σ bonds) because its negative charge is treated as a delocalized negative charge (DNC) and cannot be counted when predicting the hybridization state. The power of the hybridization state is (P_{Hyb}) = (T_{SLNC}) – 1 = 3-1 = 2 (sp^2), while the rest of the carbon atoms have an sp^2 hybridization state that corresponds to 3σ bonds (2 single bonds and 1 double bond). The presence of sp^2 hybridized carbons in cyclopropenyl anions, cyclopentadienyl anions, and cycloheptatrienyl anions make them planar.

Example C: In cyclopropenyl cations, cyclopentadienyl cations, and cycloheptatrienyl cations (Fig. 2.12, Fig. 2.13, and Fig. 2.14), the vertex carbon atoms bearing a positive charge are in an sp^2 hybridization state. In all cases, the vertex carbon atom is surrounded by 3 single bonds (σ bonds). Therefore, the power of the hybridization state is (P_{Hyb}) = (T_{SLNC}) – 1 = 3-1 = 2 (sp^2), whereas the rest of the carbon atoms have an sp^2

hybridization state that corresponds to 3σ bonds (2 single bonds and 1 double bond). The presence of sp^2 hybridized carbons in cyclopropenyl cations, cyclopentadienyl cations, and cycloheptatrienyl cations make them planar.

Example D: In cyclobutadiene and cyclooctatetraene (Fig. 2.15), all of the carbon atoms will be surrounded by 3σ bonds (2 single bonds and 1 double bond). The power of the hybridization state is $(P_{Hyb}) = (T_{SLNC}) - 1 = 3\text{-}1 = 2$ (sp^2), which makes them planar.

2. Innovative mnemonics to predict the hybridization state (sp^2 & sp^3) of the heteroatom in heterocyclic compounds

The hybridization state of a heteroatom in heterocyclic compounds can be calculated from the total number of σ bonds around it and the number of localized lone pairs of electrons (T_{SLLP}). After this, subtract 1 from this total value of T_{SLLP} to get the hybridization state (sp^2 and sp^3) of the heteroatom in heterocyclic compounds.

Example A: In Pyridine (Fig. 2.16), the lone pair of the N atom is to be treated as an LLP because it is directly attached by double and single bonds to the ring system. This means it can be used to calculate the power of the hybridization state, using $(P_{Hyb}) = (T_{SLLP}) - 1$. In pyridine, around the N, there are 2 σ bonds and 1 LLP and the power of its hybridization state is $(P_{Hyb}) = (T_{SLLP}) - 1 = (2+1)\text{-}1 = 2$ (sp^2-N). All of the other 5 carbon atoms are in the same hybridization state (sp^2); therefore, pyridine is planar.

Example B: In Pyrrole (Fig. 2.16), the lone pair from the N atom should be treated as a DLP because it is directly attached using only 3 single bonds. This means it cannot be used to calculate the power of the hybridization state. Instead, the formula, $(P_{Hyb}) = (T_{SLLP}) - 1$, should be used to predict the hybridization state. Around the N, there are 3 σ bonds and 0 LLP. The power of its hybridization state is $(P_{Hyb}) = (T_{SLLP}) - 1 = (3+0)\text{-}1 = 2$ (sp^2-N). All of the other 4 carbon atoms are in the same hybridization state (sp^2); therefore, pyrrole is planar.

Example C: In quinoline (Fig. 2.16), the lone pair of the N atom should be as an LLP because it is directly attached to the ring system with double and single bonds. This means it can be used to calculate the power of the hybridization state. The formula, $(P_{Hyb}) = (T_{SLLP}) - 1$, is used to predict the hybridization state. There are 2 σ bonds and 1 LLP. The power of the hybridization state is $(P_{Hyb}) = (T_{SLLP}) - 1 = (2+1)\text{-}1 = 2$ (sp^2-N). All of the other carbon atoms are in the same hybridization state (sp^2); therefore, quinoline is planar.

Example D: In aziridine (Fig. 2.17), the N atom is surrounded by 3 σ bonds and 1 LLP. Therefore, the power of the hybridization state is $(P_{Hyb}) = (T_{SLLP}) - 1 = (3+1) - 1 = 3$ (sp^3-N) and it is non-planar.

Examples that predict the hybridization state of heteroatoms in heterocyclic compounds have been explored in Table 2.3.

It can be expected that these time efficient innovative mnemonics will help the students of chemical education at undergraduate, senior undergraduate, and postgraduate levels to predict the hybridization state of carbon atoms and heteroatoms in organic compounds. This will enable them to detect both the planarity and aromaticity of organic compounds. Experiments, *in vitro*, on 100 students, showed that these innovative formulae could save up to 2–3 minutes in the examination hall. On the basis of this, I can strongly recommend using these nmemonics in organic chemistry.

CHAPTER 3

PREDICTION OF THE HYBRIDIZATION STATE – A COMPARATIVE STUDY BETWEEN CONVENTIONAL AND INNOVATIVE FORMULAE

The previous two chapters (Chapters 1 and 2) used formulae-based mnemonics by counting the total number of σ bonds with a lone pair of electrons (LP), a localized negative charge (LNC), or a localized lone pair of electrons (LLP) and subtracting one (−1) from this total value (T_{SLP}, T_{SLNC}, or T_{SLLP}) to predict the power of the hybridization state of simple molecules or ions and organic compounds, including heterocyclic compounds. This is an innovative and time-efficient method of enhancing student interest. These learners belong to the “paranoia zone of chemistry”. However, in this chapter, the limitations of conventional formulae in comparison to the use of innovative formulae have been discussed. Educators can use this comparative study in their classroom lectures to make chemistry intriguing.

FORMULAE

i) Conventional formulae for the prediction of the hybridization state:

The hybridization state for a molecule can be calculated using $P = 1/2\ (V+MA-C+A)$,

where V = the number of valance electrons in the central atom, MA = the number of surrounding monovalent atoms,

C = cationic charge, A = anionic charge, and P = power of the hybridization state.

ii) An innovative formula for predicting the hybridization state of simple molecules or ions:

The power of the hybridization state of the central atom is $(P_{Hyb}) = (T_{SLP}) - 1$, Where P_{Hyb} = power of the hybridization state of the central atom, T_{SLP} = (total number of σ bonds around each central atom + LP).

In order to work out a molecule's Lewis structure, first predict the number of sigma bonds (σ-bonds), pi bonds (π-bonds), and the lone pair of electrons (LP), if any. All single (-) bonds are σ bonds, while 1σ and 1π are the double bond (=), and1σ and 2π (exclude π bond) form the triple bond (≡). In addition to these, each co-ordinate bond (→) can be treated as a 1σ bond. This formula is applicable up to four (●4)T_{SLP}.

If the power of the hybridization state (P_{Hyb}) is ●3, ●2, and ●1 then the hybridization state will be sp^3, sp^2, and sp, respectively.

iii) An innovative formula for predicting the hybridization state of carbon atom in different organic compounds:

Power of the hybridization state in the central atom, (P_{Hyb}) = (T_{SLNC}) – 1

Where P_{Hyb} = power of the hybridization state of the central atom, and T_{SLNC} = (total number of σ bonds around each central atom + localized negative charge).

All single (-) bonds are σ bonds, while 1σ and 1π are the double bond (=). Also, (LNC) = localized negative charge. A negative charge bearing carbon atom in the ring system of the organic compound when directly attached with single and double bonds is considered to be an LNC containing carbon atom and its negative charge is to be treated accordingly.

iv) An innovative formula for predicting the hybridization state of the heteroatom in different heterocyclic compounds:

Power of the hybridization state of a heteroatom (P_{Hyb}) = (T_{SLLP}) – 1,

Where P_{Hyb} = power of the hybridization state of the heteroatom, T_{SLLP} = (total number of σ bonds around each central atom + LLP), and LLP = localized lone pair of electrons. If the power of the hybridization state (P_{Hyb}) is ●3, ●2, and ●1 then the hybridization state will be sp^3, sp^2, and sp, respectively. All single (-) bonds are σ bonds, while in a double bond (=) there is one σ and one π. The heteroatom (an atom containing a lone pair of electrons), which is directly attached with single and double bonds using the ring system, is considered to be an LLP-based heteroatom and its lone pair is to be treated as a localized lone pair of electrons (LLP).

RESULTS AND DISCUSSION

This was a comparative study between conventional and innovative formulae for the prediction of the hybridization state of different atoms in simple molecules or ions.

When using a conventional formula, it is not possible to predict the hybridization state of an O atom in the cyclic ozone (Fig. 1.2).

Example 1: The hybridization state of O in cyclic ozone

Conventional formula: $P = 1/2\ (V+MA-C+A) = 1/2\ (6+0-0) = 3.0$ (sp^2-erroneous hybridization state of O)

Innovative formula: $(P_{Hyb}) = (T_{SLP}) - 1 = (2+2)-1 = 3$ (sp^3 hybridized O atom in cyclic ozone)

Where P_{Hyb} = power of the hybridization state of the central atom, and T_{SLP} = (total number of σ bonds around each central atom + LP)

It is not possible to predict the hybridization state of the S atom in S_8 and the P atom in P_4 (Fig. 1.4) using a conventional formula.

Example 2: The hybridization state of S in S_8

Conventional formula: $P = 1/2\ (V+MA-C+A) = 1/2\ (6+0-0) = 3.0$ (sp^2-erroneous hybridization state of S in S_8)

Innovative formula: $(P_{Hyb}) = (T_{SLP}) - 1 = (2+2)-1 = 3$ (sp^3 hybridized S atom in S_8)

Where P_{Hyb} = power of the hybridization state of the central atom, and T_{SLP} = (total number of σ bonds around each central atom + LP)

Example 3: The hybridization state of P in P_4

Conventional formula: $P = 1/2\ (V+MA-C+A) = 1/2\ (5+0-0) = 2.5$ (unpredictable hybridization state of P in P_4)

Innovative formula: $(P_{Hyb}) = (T_{SLP}) - 1 = (3+1)-1 = 3$ (sp^3 hybridized P atom in P_4),

Where P_{Hyb} = power of the hybridization state of the central atom, T_{SLP} = (total number of σ bonds around each central atom + LP)

It is not possible to predict the hybridization state of a terminal carbon atom in alkynes using a conventional formula.

Example 4: The hybridization state of Ethyne (Fig. 3.18).

Conventional formula: $P = 1/2\,(V+MA-C+A) = 1/2\,(4+1-0) = 2.5$ (unpredictable hybridization state).

Innovative formula: $(P_{Hyb}) = (T_{SLP}) - 1 = 2-1 = 1$ (sp hybridized carbon atom in alkyne),

where P_{Hyb} = power of the hybridization state of the central atom, T_{SLP} = (total number of σ bonds around each central atom + LP)

Example 5: The hybridization state of pent-1-ene-4-yne (Fig. 3.19).

Conventional formula: power of the hybridization state of the terminal carbon

$C_5(P) = 1/2\,(V+MA-C+A) = 1/2\,(4+1-0) = 2.5$ (unpredictable hybridization state C_5).

Innovative formula: (P_{Hyb}) for $C_5 = (T_{SLP}) - 1 = 2-1 = 1$ (sp hybridized C_5),

Where P_{Hyb} = power of the hybridization state of the central atom, T_{SLP} = (total no of σ bonds around each central atom + LP)

It is not possible to predict the hybridization state of oxygen atoms in the cyclic ozone or hydrogen peroxide, the S atom in S_8, or the P atom in P_4 using a conventional formula; however, using an innovative formula allows the hybridization state to be determined with absolute accuracy in all cases.

A comparative study between conventional and innovative formulae to predict the hybridization state of carbon atoms in different non-heterocyclic organic compounds

It is not possible to predict the hybridization state of carbon atoms in cyclopropene, cyclopentadiene, cycloheptatriene, cyclopropenyl anion, cyclopentadienyl anion, cycloheptatrienyl anion, cyclopropenyl cation, cyclopentadienyl cation, and cycloheptatrienyl cation, benzene, and toluene using a conventional formulae; however, using an innovative formula allows the hybridization state to be determined with absolute accuracy in all cases.

When a conventional formula was used the hybridization state of a vertex carbon atom in cycloalkenes, such as cyclopropene, cyclopentadiene, and cycloheptatriene (Fig. 2.12, Fig. 2.13, and Fig. 2.14), it gave erroneous results.

i) Conventional formula

The power of the hybridization state of the vertex carbon (P) = 1/2 (V+MA−C+A) = 1/2 (4+2-0) = 3 (sp^2- erroneous hybridization state).

ii) Innovative formula

Power of the hybridization state, (P_{Hyb}) = (T_{SLNC}) – 1 = 4-1 = 3 (sp^3 hybridization state of vertex carbon).

The hybridization state of carbon atoms, other than vertex carbon, in cycloalkenes, such as cyclopropene, cyclopentadiene and cycloheptatriene (Fig. 2.12, Fig. 2.13, and Fig. 2.14), was unpredictable when using a conventional formula.

i) Conventional formula

The power of the hybridization state of the rest carbons (P) = 1/2 (V+MA–C+A) = 1/2 (4+1-0) = 2.5

(unpredictable hybridization state).

ii) Innovative formula

The power of the hybridization state was (P_{Hyb}) = (T_{SLNC}) – 1 = 3-1 = 2

(sp^2 hybridization state of rest carbons other than vertex carbon).

The hybridization state of vertex carbon atoms bearing a negative charge in cycloalkenyl anions, such as cyclopropenyl anion, cyclopentadienyl anion, and cycloheptatrienyl anion (Fig. 2.12, Fig. 2.13, Fig. 2.14),was erroneous when using a conventional formula.

i) Conventional formula

The power of the hybridization state of the vertex carbon (P) = 1/2 (V+MA–C+A) = 1/2 {4+1-(0-1)} = 1/2{6} = 3

(sp^2 - erroneous hybridization state).

ii) Innovative formula

The power of the hybridization state of the vertex carbon is $(P_{Hyb}) = (T_{SLNC}) - 1 = 3\text{-}1 = 2$ (sp^2 hybridization state).

The hybridization state of a vertex carbon atom bearing a positive charge in cycloalkenyl cations, such as cyclopropenyl cation, cyclopentadienyl cation, and cycloheptatrienyl cation (Fig. 2.12, Fig. 2.13, Fig. 2.14), was erroneous when using a conventional formula.

i) Conventional formula

The power of the hybridization state in a vertex carbon bearing a positive charge, $(P) = 1/2\ (V+MA-C+A) = 1/2\ \{4+1\text{-}(1+0)\}$

$= 1/2\{4\} = 2$ (sp - erroneous hybridization state).

ii) Innovative formula

Power of the hybridization state of the vertex carbon bearing positive charge, $(P_{Hyb}) = (T_{SLNC}) - 1 = 3\text{-}1 = 2$ (sp^2 hybridization state).

The hybridization state of carbon atoms in benzene, toluene, and so on is unpredictable using a conventional formula but, when using an innovative formula, the hybridization state will be determined with absolute accuracy in all cases.

A carbon atom in benzene (Fig. 3.20)

i) Conventional formula

The power of the hybridization state of carbon is $(P) = 1/2\ (V+MA-C+A) = 1/2\ (4+1\text{-}0) = 2.5$ (unpredictable hybridization state).

ii) Innovative formula

The power of the hybridization state of a carbon atom is $(P_{Hyb}) = (T_{SLNC}) - 1 = 3\text{-}1 = 2$ (sp^2 hybridization state).

Carbon atom from the methyl group in Toluene (Fig. 3.20)

i) Conventional formula

The power of the hybridization state of a carbon atom from the methyl group in toluene is

$(P) = 1/2\ (V+MA-C+A) = 1/2\ (4+3-0) = 3.5$ (unpredictable hybridization state).

ii) Innovative formula

The power of the hybridization state of a carbon atom from the methyl group in toluene is

$(P_{Hyb}) = (T_{SLNC}) - 1 = 4-1 = 3$ (sp^3 hybridization state).

A comparative study between conventional and innovative formulae to predict the hybridization state of a heteroatom in different heterocyclic compounds

It is not possible to predict the hybridization state of heteroatom nitrogen in pyridine, quinoline, isoquinoline, pyrimidine, thiazole, benzothiazole, pyrazine, cyanidine, phenazine, 1,2,3,4-tetrazine, azocine, azetine, and aziridine, or an oxygen atom in oxetan using a conventional formula. However, when using an innovative formula, the hybridization state of a heteroatom in nitrogen will be determined with absolute accuracy in all cases.

i) Conventional formula

The power of the hybridization state of a nitrogen atom in pyridine is $P = 1/2\ (V+MA-C+A) = 1/2\ (5 + 0 - 0 + 0) = 2.5$ (unpredictable hybridization state) and the power of the hybridization state of a nitrogen atom in quinolone is $P = 1/2\ (V+H-C+A) = 1/2\ (5 + 0 - 0 + 0) = 2.5$ (unpredictable hybridization state) (Fig. 2.16).

The power of the hybridization state of a nitrogen atom in aziridin is $P = 1/2\ (V+MA-C+A) = 1/2\ (5 + 1 - 0 + 0) = 3$ (sp^2– erroneous hybridization state of N) and the power of the hybridization state of an oxygen atom in oxetan is $P = 1/2(V+MA-C+A) = 1/2\ (6 + 0 - 0 + 0) = 3$ (sp^2- erroneous hybridization state of oxygen atom) (Fig. 2.17).

ii) Innovative formula

The power of the hybridization state of a heteroatom is (P_{Hyb}) = (T_{SLLP}) – 1.

The power of the hybridization state of a nitrogen atom in pyridine is P_{Hyb} = (3 - 1) = 2 (σ bonds = 2 & LLP = 1)

(sp^2 hybridization state of N atom) and the power of the hybridization state of a nitrogen atom in quinolone is P_{Hyb} = (3 -1) = 2 (σ bonds = 2 & LLP = 1) (sp^2 hybridization state of N atom) (Fig. 2.16).

The power of the hybridization state of a nitrogen atom in aziridine is P_{Hyb} = (4 - 1) = 3 (σ bonds = 3 & LLP = 1)

sp^3 hybridization state of N atom) and the power of the hybridization state of an oxygen atom in oxetan is P_{Hyb} = (4 - 1) = 3 (σ bonds = 2 & LLP = 2) (sp^3 hybridization state of O atom) (Fig. 2.17).

In this chapter, the limitations of conventional formulae have been discussed in the light of innovative formulae to predict the hybridization state of simple molecules or ions and organic compounds, including heterocyclic compounds. Educators can use this comparative study in their classroom lectures to make chemistry intriguing and trustworthy.

CHAPTER 4

INNOVATIVE MNEMONICS FOR THE PREDICTION OF THE BOND ORDER OF DIATOMIC SPECIES WITHOUT MOLECULAR ORBITAL THEORY (MOT)

In Chapters 1 and 2, formulae-based mnemonics were discussed to predict the power of the hybridization state of simple molecules or ions, carbon atoms in organic compounds, and heteroatoms in heterocyclic compounds. The limitations of conventional formulae were the focus of Chapter 3. In this chapter, the bond order of diatomic species with 1–20 electrons will be predicted without drawing a molecular orbital diagram or using molecular orbital theory. I will present 4 time efficient innovative mnemonics to predict the bond order of diatomic species. I will also discuss the use of bond orders in chemical bonding, as well as the different problems associated with it. This chapter explores the results and provides suggestions for context-based teaching, learning, and assessment. The bond order is usually predicted by using MOT, which was first proposed by Friedrich Hund and Robert Mulliken in 1933.[6] They developed an approach to the covalent bond formation based upon the effects of various electron fields. This uses a molecular orbital rather than an atomic orbital. Each orbital characterizes the molecule as a whole, which has a definite combination of quantum numbers and a relative energy value.

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[6] R. S. Mulliken, *Spectroscopy, Molecular Orbitals, and Chemical Bonding Nobel Lectures Chemistry* (Amsterdam Elsevier Publishing Company: 1972), 1963 1970; George G. Hall, "The Lennard-Jones Paper of 1929 and the foundations of Molecular Orbital Theory", *Advances in Quantum Chemistry* 22 (1991): 1 6, doi:10.1016/S0065-3276(08)60361-5.

METHODOLOGY

A. The conventional method to predict the bond order (MOT)

According to MOT, in a molecule, all atomic orbitals from participating atoms overlap or mix up to form an equivalent number of new orbitals called molecular orbitals. In doing so, the atomic orbitals lose their individual identity and all the electrons get distributed in the molecular orbital in accordance with Aufbau's principle, Pauli's exclusion principle, and Hund's rule. The formation of molecular orbitals is explained using the linear combination of atomic orbitals (LACO). When atomic orbitals approach each other, their wave functions (ψ) interact with each other in two different ways:

i) Bonding molecular orbital (BMO): Constructive interference; this is when two waves are in a phase and produce an additive effect, which creates a bonding molecular orbital (BMO).

ii) Anti-bonding molecular orbital (ABMO): Destructive interference; this is when two waves are out of sync and produce a subtractive effect, which creates an anti-bonding molecular orbital (ABMO).

BMOs are formed by the addition of atomic orbitals and are represented by σ, π, and so on. The energy of BMOs is lower than that of combining atomic orbitals. ABMOs are formed by subtracting atomic orbitals and are represented by σ^*, π^*, and so on. The energy of ABMOs is higher than that of combining atomic orbitals. ABMOs are higher in energy than their corresponding BMOs. Therefore, BMOs are more stable than ABMOs. Electrons have a lower energetic BMO by obeying Hund's rule and a corresponding higher energy ABMO. The probability of finding electrons increases in BMO, but decreases in ABMO.

The atomic orbitals, which do not take part in bond formation, are known as non-bonding orbitals. For example, in HF, sigma bonding and anti-bonding orbitals are formed by combining 1s orbital on an H-atom with the $2p_z$ orbital on a fluorine (F) atom. This is why, 1s, 2s, $2p_x$, and $2p_y$ orbitals on fluorine (F) remain non-bonding orbitals.

Increasing energetic order of different molecular orbitals for electrons ≤ 14

$$\sigma_{1s} < \sigma^*_{1s} < \sigma_{2s} < \sigma^*_{2s} < \pi_{2Px} = \pi_{2py} < \sigma_{2pz} < \pi^*_{2px} = \pi^*_{2py} < \sigma^*_{2pz}$$

Increasing energetic order of different molecular orbitals for electrons > 14

$$\sigma_{1s} < \sigma^*_{1s} < \sigma_{2s} < \sigma^*_{2s} < \sigma_{2pz} < \pi_{2Px} = \pi_{2py} < \pi^*_{2px} = \pi^*_{2py} < \sigma^*_{2pz}$$

In this energetic order, there are 5 bonding molecular orbitals (BMOs), σ_{1s}, σ_{2s}, π_{2px}, π_{2py}, σ_{2pz} and five anti-bonding molecular orbitals (ABMOs), σ^*_{1s}, σ^*_{2s}, π^*_{2px}, π^*_{2py}, σ^*_{2pz}.

iii) Bond Order (BO): The number of covalent bonds formed in a molecule is called its bond order. Mathematically, it is represented as $BO = N_b - N_a / 2$

Where, N_b = number of electrons in bonding molecular orbital and N_a = number of electrons in anti-bonding molecular orbitals.

If, $N_b > N_a$, then BO = +ve, the molecule is stable and if, $N_b < N_a$, then BO = -ve, the molecule is unstable or does not exist. If, $N_b = N_a$, BO = 0, the molecule does not exist.

B. Innovative mnemonics to predict the bond order without molecular orbital theory

First of all, classify the molecules or ions with 1–20 e^-s into the following 4 types, 1–2, 2–6, 6–14 and 14–20 based on the total number of electrons present.

The graphical representation (Fig. 4.21) shows that bond order gradually increases to 1 in the range 0–2 electrons, then falls to 0 in the range 2–4 electrons, then it rises to 1 for 4–6 electrons and falls to 0 for 6–8 electrons, then again rises to 3 in the range 8–14 electrons and finally falls to 0 for 14–20 electrons. For electrons numbered 2, 6, and 14, one can use multiple formulae because they overlap. For the 4 divisions, there will be 4 formulae used to predict the bond order of homo and heteronuclear diatomic molecules or ions with 1–20[7] electrons.

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[7] A. Das, "Bond-order and Magnetic Behavior of Diatomic Species without Molecular Orbital Theory", *World Journal of Chemical Education* 5 (June 2017): 128 131, doi: 10.12691/wjce-5-4-2, http://pubs.sciepub.com/wjce/5/4/2/; A. Das, “Innovative Mnemonics in Chemical Education: A Review Article”, *American Journal of Chemistry and Applications* 5 (April 2018): 19-32, http://www.openscienceonline.com/journal/archive2?journalId=711&paperId=4221; A. Das, “A Review of Time Economic Innovative Mnemonics in Chemical

i) Molecules and ions with 1–2 electrons:

Bond order = n/2

ii) Molecules and ions with a total number of electrons within the range 26:

Bond order = I 4 - n I / 2

iii) Molecules and ions with 6–14 electrons:

Bond order = I 8 - n I / 2

iv) Molecules and ions with 14–20 electrons:

Bond order = (20 - n) / 2

[where n = total no of electrons, II indicates Mod function and so the value of bond order is always positive]

By just using the total number of electrons (n), the bond order of the diatomic species should easily be predicted without using MOT.

RESULTS AND DISCUSSION

A. Predicting the bond order using the conventional method:

Example: H_2 (number of electrons < 14)**:** Electronic configuration (EC) with MOT σ_{1s}^2, BO = $N_b - N_a / 2$ = 2-0/2 = 1 (H-H); **H_2^+**: EC with MOT σ_{1s}^1, BO = $N_b - N_a / 2$ = 1-0/2 = 0.5; **H_2^-**: EC with MOT σ_{1s}^2, $\sigma^*_{1s}{}^1$, BO = $N_b - N_a / 2$ = 2-1/2 = 0.5.

Education", *International Journal of Physics & Chemistry Education* 10 (June 2018):27 40, doi: 10.12973/ijpce/81589, http://www.ijpce.org/A-Review-of-Time-Economic-Innovative-Mnemonics-in-Chemical-Education,81589,0,2.html; A. Das, "Innovative Mnemonics in Chemical Education: Review Article", *African Journal of Chemical Education* 8(July 2018): 144 189, https://www.ajol.info/index.php/ajce/article/view/176086; A. Das, "Innovative Mnemonics Make Chemical Education Time Economic: A Pedagogical Review Article", *World Journal of Chemical Education* 6 (Sept 2018): 154 174, doi:10.12691/wjce-6-4-2, http://pubs.sciepub.com/wjce/6/4/2/index.html; A. Das, "Chemical Bonding: Time Economic Innovative Pedagogies - A Review Article", *Global Journal of Science Frontier Research Chemistry* 17 (Nov 2017): 1 16, https://journalofscience.org/index.php/GJSFR/article/view/2110.

He_2: EC is σ_{1s}^2, $\sigma^{*}{}_{1s}^{2}$, $BO = N_b - N_a/2 = 2-2/2 = 0$ (does not exist); **He_2^+**: EC is σ_{1s}^2, $\sigma^{*}{}_{1s}^{1}$, $BO = N_b - N_a/2 = 2-1/2 = 0.5$.

Li_2: EC is σ_{1s}^2, $\sigma^{*}{}_{1s}^{2}$, σ_{2s}^2, $BO = N_b - N_a/2 = 4-2/2 = 1$; **$Be_2$**: EC is σ_{1s}^2, $\sigma^{*}{}_{1s}^{2}$, σ_{2s}^2, $\sigma^{*}{}_{2s}^{2}$, $BO = N_b - N_a/2 = 4-4/2 = 0$ (does not exist); **B_2**: EC is σ_{1s}^2, $\sigma^{*}{}_{1s}^{2}$, σ_{2s}^2, $\sigma^{*}{}_{2s}^{2}$, π_{2px}^1, π_{2py}^1 (Fig. 4.22), bond order $= N_b - N_a/2 = 6-4/2 = 1$ (B-B); **C_2**: EC is σ_{1s}^2, $\sigma^{*}{}_{1s}^{2}$, σ_{2s}^2, $\sigma^{*}{}_{2s}^{2}$, π_{2px}^2, π_{2py}^2, bond order $= N_b - N_a/2 = 8-4/2 = 2$ (C=C).

N_2: EC is σ_{1s}^2, $\sigma^{*}{}_{1s}^{2}$, σ_{2s}^2, $\sigma^{*}{}_{2s}^{2}$, π_{2px}^2, π_{2py}^2, σ_{2pz}^2, bond order $= N_b - N_a/2 = 10-4/2 = 3$ (N≡N); **N_2^+**: EC is σ_{1s}^2, $\sigma^{*}{}_{1s}^{2}$, σ_{2s}^2, $\sigma^{*}{}_{2s}^{2}$, π_{2px}^2, π_{2py}^2, σ_{2pz}^1, bond order $= N_b - N_a/2 = 9-4/2 = 2.5$; **$N_2^-$** : EC is σ_{1s}^2, $\sigma^{*}{}_{1s}^{2}$, σ_{2s}^2, $\sigma^{*}{}_{2s}^{2}$, π_{2px}^2, π_{2py}^2, σ_{2pz}^2 , $\pi^{*}{}_{2px}^{1}$, bond order $= N_b - N_a/2 = 10-5/2 = 2.5$; **$N_2^{2-}$** : EC is σ_{1s}^2, $\sigma^{*}{}_{1s}^{2}$, σ_{2s}^2, $\sigma^{*}{}_{2s}^{2}$, π_{2px}^2, π_{2py}^2, σ_{2pz}^2 , $\pi^{*}{}_{2px}^{1}$, $\pi^{*}{}_{2py}^{1}$, bond order $= N_b - N_a/2 = 10-6/2 = 2$.

O_2 (number of electrons > 14): EC of O_2 is σ_{1s}^2, $\sigma^{*}{}_{1s}^{2}$, σ_{2s}^2, $\sigma^{*}{}_{2s}^{2}$, σ_{2pz}^2, π_{2px}^2, π_{2py}^2, $\pi^{*}{}_{2px}^{1}$, $\pi^{*}{}_{2py}^{1}$ (Fig. 4.23), $BO = N_b - N_a/2 = 10-6/2 = 2$ (O=O); **O_2^+**: EC is σ_{1s}^2, $\sigma^{*}{}_{1s}^{2}$, σ_{2s}^2, $\sigma^{*}{}_{2s}^{2}$, σ_{2pz}^2, π_{2px}^2, π_{2py}^2, $\pi^{*}{}_{2px}^{1}$, $BO = N_b - N_a/2 = 10-5/2 = 2.5$; **$O_2^-$**: EC is σ_{1s}^2, $\sigma^{*}{}_{1s}^{2}$, σ_{2s}^2, $\sigma^{*}{}_{2s}^{2}$, σ_{2pz}^2, π_{2px}^2, π_{2py}^2, $\pi^{*}{}_{2px}^{2}$, $\pi^{*}{}_{2py}^{1}$, $BO = N_b - N_a/2 = 10-7/2 = 1.5$; **$O_2^{2-}$** : EC is σ_{1s}^2, $\sigma^{*}{}_{1s}^{2}$, σ_{2s}^2, $\sigma^{*}{}_{2s}^{2}$, σ_{2pz}^2, π_{2px}^2, π_{2py}^2, $\pi^{*}{}_{2px}^{2}$, $\pi^{*}{}_{2py}^{2}$, $BO = N_b - N_a/2 = 10-8/2 = 1$.

F_2: EC is σ_{1s}^2, $\sigma^{*}{}_{1s}^{2}$, σ_{2s}^2, $\sigma^{*}{}_{2s}^{2}$, σ_{2pz}^2, π_{2px}^2, π_{2py}^2, $\pi^{*}{}_{2px}^{2}$, $\pi^{*}{}_{2py}^{2}$, $BO = N_b - N_a/2 = 10-8/2 = 1$ (F-F).

Ne_2: EC is σ_{1s}^2, $\sigma^{*}{}_{1s}^{2}$, σ_{2s}^2, $\sigma^{*}{}_{2s}^{2}$, σ_{2pz}^2, π_{2px}^2, π_{2py}^2, $\pi^{*}{}_{2px}^{2}$, $\pi^{*}{}_{2py}^{2}$, $\sigma^{*}{}_{2pz}^{2}$, $BO = N_b - N_a/2 = 10-10/2 = 0$ (does not exist).

CN (number of electrons < 14): EC is σ_{1s}^2, $\sigma^{*}{}_{1s}^{2}$, σ_{2s}^2, $\sigma^{*}{}_{2s}^{2}$, π_{2px}^2, π_{2py}^2, σ_{2pz}^1, bond order $= N_b - N_a/2 = 9-4/2 = 2.5$; **$CN^-$**: EC is σ_{1s}^2, $\sigma^{*}{}_{1s}^{2}$, σ_{2s}^2, $\sigma^{*}{}_{2s}^{2}$, π_{2px}^2, π_{2py}^2, σ_{2pz}^2, bond order $= N_b - N_a/2 = 10-4/2 = 3$.

NO (number of electrons > 14): EC is σ_{1s}^2, $\sigma^{*}{}_{1s}^{2}$, σ_{2s}^2, $\sigma^{*}{}_{2s}^{2}$, σ_{2pz}^2, π_{2px}^2, π_{2py}^2, $\pi^{*}{}_{2px}^{1}$, $BO = N_b - N_a/2 = 10-5/2 = 2.5$; **$NO^+$**: EC is σ_{1s}^2, $\sigma^{*}{}_{1s}^{2}$, σ_{2s}^2, $\sigma^{*}{}_{2s}^{2}$, σ_{2pz}^2, π_{2px}^2, π_{2py}^2, $BO = N_b - N_a/2 = 10-4/2 = 3$.

B. Predicting the bond order of B_2 (total electrons = 10) and O_2 (total electrons = 16) using an innovative method:

Bond order of B_2: B_2 with a total number of electrons =10 (total number of electrons, n=10); therefore, it falls in the range 6–14 electrons and the bond order $= |8 - n|/2 = |8 - 10|/2 = 1$ (B-B).

Bond order of O_2: O_2 with a total number of electrons =16 (total number of electrons, n=16); therefore, it falls in the range 14–20 electrons and the bond order = 20 - n/2 = 20-16/2 = 2 (O=O).

So, with the help of innovative mnemonics, the bond order of diatomic species can easily be calculated from the total number of electrons and without drawing a molecular orbital diagram. Adequate examples on the prediction of bond order of homo and heteronuclear diatomic molecules and ions with 1–20 electrons have been explored in Table 4.4.

THE APPLICATIONS FOR BOND ORDER IN CHEMICAL EDUCATION

1. From the bond order, different parameters, such as length, strength, dissociation energy, energy, ionization energy, thermal stability, and reactivity, can also be evaluated:

i) Bond order (BO) $\propto$ 1/bond length or bond distance ii) BO $\propto$ bond strength iii) O $\propto$ bond dissociation energy iv) BO $\propto$ bond energy v) BO $\propto$ ionization energy vi) BO $\propto$ 1/reactivity vii) BO $\propto$ thermal stability viii) BO $\propto$ vibrational frequency.

Example: Bond order values of O_2, O_2^-, O_2^{2-}, O_2^+, and O_2^{2+} are 2.0, 1.5, 1.0, 2.5, and 3.0, respectively. Therefore, the decreasing order of length, strength, dissociation energy, energy, ionization energy, thermal stability, reactivity, and vibrational frequency is O_2^{2+} (3.0) > O_2^+ (2.5) > O_2 (2.0) > O_2^- (1.5) > O_2^{2-} (1.0) and the decreasing order of bond length and reactivity is O_2^{2-} (1.0) > O_2^-(1.5) > O_2 (2.0) > O_2^+ (2.5) > O_2^{2+} (3.0).

2. When the bond order of cationic (X_2^+) and anionic species (X_2^-) is the same for each element (X_2), then the anionic species (X_2^-) will be more reactive and less stable than the cationic species (X_2^+). This is due to the increasing number of electrons in the higher energy anti-bonding molecular orbital (ABMO) in the anionic species (X_2^-).

Example A: If the bond order of N_2^+ and N_2^- is 2.5, then their reactivity order will be $N_2^- > N_2^+$ and stability order will be $N_2^+ > N_2^-$.

Example B: If the bond order of H_2^+ and H_2^- is 0.5, then their reactivity order will be $H_2^- > H_2^+$ and stability order will be $H_2^+ > H_2^-$.

THE APPLICATION OF BOND ORDER MNEMONICS WHEN DESIGNING CBL ACTIVITIES

Mnemonics can be used in computer-based learning (CBL) activities and to develop chemistry educational software tools, such as the "Diatomic Bond Order Calculator".[8] This tool encourages educators, scholars, and chemistry students to solve bond order related chemistry problems. In general, students who know how to write computer programs to solve chemistry problems have an edge when taking quantitative courses, such as analytical chemistry, instrumental analysis, chemometrics, and computational chemistry. They are also better prepared for multidisciplinary research and postdoctoral work.

QUESTIONS ON BOND ORDER: (Using Bond Order Mnemonics to Solve Problems in Competitive Exams)

Q.1. Which one of these will have the highest bond order? (NEET 2018)

a) CN^+ b) CN^- c) NO d) CN

Ans: (b) CN^- (Total electrons n = 6 + 7 + 1 = 14, BO = I 8-n I / 2 = I 8-14 I / 2 = 3)

Q.2. According to molecular orbital theory, which of the following will not be a viable molecule? (JEE MAIN 2018)

a) He_2^{2+} b) He_2^+ c) H_2^- d) H_2^{2-}

Ans: (d) H_2^{2-} (Total electrons n = 4, BO = I4-nI / 2 = I4-4I 2 = 0, therefore it does not exist)

Q.3. Which one of the following pairs of species has the same bond order? (NEET 2017)

a) O_2, NO^+ b) CN^-, CO c) N_2, O_2^- d) CO, NO

Ans: (b) CN^- and CO both have BO 3.0.w.r.t. (total electrons 14)

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[8] A. Das and E. Garcia, 'Diatomic Bond Order Calculator', *minerazzi.com* (Dec 2018): http://www.minerazzi.com/tools/bond-order/calculator.php

Q.4. Decreasing order of stability of O_2, O_2^-, O_2^+ and O_2^{2-} is (NEET 2015)

a) $O_2^{2-} > O_2^- > O_2 > O_2^+$ b) $O_2 > O_2^+ > O_2^{2-} > O_2^-$ c) $O_2^- > O_2^{2-} > O_2^+ > O_2$ d) $O_2^+ > O_2 > O_2^- > O_2^{2-}$

Ans: (d) O_2^+ (2.5) > O_2 (2.0) > O_2^- (1.5) > O_2^{2-} (1.0) (BO $\propto$ stability)

Q.5. Both species will not exist in which of the following pairs of molecules/ions?

a) H_2^+, He_2^{2-} b) H_2^-, He_2^{2-} c) H_2^{2+}, He_2 d) H_2^-, He_2^{2+} (JEE MAIN 2013)

Ans: (c) (BO of $He_2 = 0$) (species with a 0 or negative bond order do not exist)

Q.6. Using MOT, predict which of the following species has the shortest bond length?

a) O_2^{2+} b) O_2^+ c) O_2^- d) O_2^{2-} (AIEEE-2009)

Ans: (a) BO of $O_2^{2+} = 3.0$; BO $\propto$ 1/bond length)

Q.7. Which molecule/ion has a bond order of 2.5? (S.T.P.G.T. 2017)

a) Li_2^+ b) F_2^+ c) O_2^+ d) C_2

Ans: (c) ($O_2^+ = 2.5$)

Q.8. Using MOT t, predict which of the following species will have the shortest bond length?

a) O_2^{2+} b) O_2^+ c) O_2^- d) O_2^{2-} (AIEEE 2009)

Ans: (a) O_2^{2+} (BO = 3, BO $\propto$ 1/bond length)

Q.9. The stability of the species increases in which order? (JEE MAIN 2013)

a) $Li_2 < Li_2^+ < Li_2^-$ b) $Li_2^- < Li_2^+ < Li_2$ c) $Li_2 < Li_2^- < Li_2^+$ d) $Li_2^- < Li_2 < Li_2^+$

Ans: (b) $Li_2^- < Li_2^+ < Li_2$

(Li_2 = BO = 1, Li_2^+ & Li_2^- BO = 0.5; the bond order has a stability of $\propto$ but when the bond order is the same then the cationic species will have a greater stability than anionic species due to an increase in electrons with a higher energy ABMO)

Q.10. Among the following species, the order of ionization energy (IE_1) is

a) $O_2<O_2^+<O_2^-$ b) $O_2^+<O_2^-<O_2$ c) $O_2^-<O_2<O_2^+$ d) $O_2<O_2^-<O_2^+$

Ans: (c) $O_2^-<O_2<O_2^+$ - IE_1 (bond order $\propto$ IE_1; the bond order trend is $1.5<2.0<2.5$)

Q.11. Which is the correct order of stability?

a) $CN < NO^+ < NO^-$ b) $NO^- < CN < NO^+$ c) $NO^+ < CN < NO^-$ d) $CN < NO^- < NO^+$

Ans: (b) NO^- (2.0) < CN (2.5) < NO^+ (3.0) - stability (bond order $\propto$ stability)

Q.12. When does the bond order increase?

a) O_2 changes to O_2^+ b) N_2 changes to N_2^+ c) NO changes to NO^- d) In all of the above

Ans: (a) O_2 changes to O_2^+ (bond order increases from 2.0 to 2.5)

Q.13. Which of the following is the correct order of stability?

a) $N_2>N_2^+>N_2^-$ b) $N_2> N_2^->N_2^+$ c) $N_2^+ >N_2>N_2^-$ d) None of the above

Ans: (a) $N_2>N_2^+>N_2^-$ (bond order $N_2 = 3.0$, N_2^+ & $N_2^- = 2.5$; bond order $\propto$ stability)

Q.14. According to molecular orbital theory, which of the following does not exist?

a) H_2^- b) O_2^- c) He_2 d) O_2^+

Ans: (c) He_2 (BO = 0)

Q.15. Which molecular species has the highest bond order?

a) O_2 b) O_2^- c) O_2^+ d) O_2^{2-}

Ans: (c) O_2^+ (BO = 2.5)

Q.16. N_2 and O_2 are converted into monocations, N_2^+ and O_2^-, respectively. Which is incorrect?

a) in N_2^+, the N-N bond is weakened b) in O_2^+, the O-O bond is increased c) in O_2^+, paramagnetism is decreased d) N_2^+ becomes diamagnetic

Ans: (d) N_2^+; it becomes paramagnetic rather than diamagnetic

Q.17. The calculated bond order in H_2^- ion is

a) 0 b) 1/2 c) -1/2 d) 1

Ans: (b) 1/2

Q.18. Which is the correct bond order sequence?

a) $O_2^+ > O_2^- > O_2$ b) $O_2 > O_2^- > O_2^+$ c) $O_2^+ > O_2 > O_2^-$ d) $O_2^- > O_2^+ > O_2$

Ans: (c) $O_2^+ > O_2 > O_2^-$ (BO 2.5 > 2.0 > 1.5)

Q.19. Which molecule has a bond order of 3?

a) H_2 b) N_2 c) O_2 d) He_2^+

Ans: (b) N_2 (BO = 3)

Q.20. What is the relationship between the dissociation energy of N_2 and N_2^+?

a) The dissociation energy of N_2 = dissociation energy of N_2^+ b) The dissociation energy of N_2 can either be lower or higher than the dissociation energy of N_2^+ c) The dissociation energy of N_2 > dissociation energy of N_2^+ d) The dissociation energy of N_2 < dissociation energy of N_2^+

Ans: (c) The dissociation energy of N_2 > dissociation energy of N_2^+ (BO $\propto$ dissociation energy; BO of N_2 is 3.0 and that of N_2^+ is 2.5)

Q.21. What forms an antibonding molecular orbital?

a) addition of atomic orbitals b) subtraction of atomic orbitals c) multiplication of atomic orbitals d) None of the above.

Ans: (b) Subtraction of atomic orbitals gives rise to anti-bonding molecular orbitals

Q.22. A bonding molecular orbital is formed by the

a) addition of atomic orbitals b) subtraction of atomic orbitals c) division of atomic orbitals d) None of the above.

Ans: (a) The addition of atomic orbitals gives rise to bonding molecular orbitals

Q.23. The bond order of O_2^- is

a) 0.5 b) 1.5 c) 3.5 d) 2.5

Ans: (b) 1.5

Q.24. The number of anti-bonding electron pairs on an O_2^{2-} molecular ion using MOT is

a) 4 b) 3 c) 2 d) 5

Ans: (a) 4 (EC of O_2^{2-} is σ_{1s}^2, $\sigma^*_{1s}{}^2$, σ_{2s}^2, $\sigma^*_{2s}{}^2$, σ_{2pz}^2, π_{2px}^2, π_{2py}^2, $\pi^*_{2px}{}^2$, $\pi^*_{2py}{}^2$)

Q.25.The common features among the species CN^-, CO, and NO^+ are

a) bond order 3 and isoelectronic b) bond order 3 and weak field ligands c) bond order 3 and π-acceptors d) isoelectronic and weak field ligands

Ans: (a) bond order 3 and isoelectronic (all have 14 electrons and a BO of 3)

Q.26. Two sp^3 hybridized carbons are present in which of the following compounds?

a) $CH_3CH=CH_2$ b) CH_3CH_2OH c) CH_3CHO d) CH_3COOH

Ans: (b) CH_3CH_2OH (both carbon atoms are surrounded by 4σ bonds and are sp^3 hybridized)

Q.27. Match column I with column II, and then select the correct answer using the code given below.

Column I (Molecule/Ion)	**Column II (Molecular Geometry)**
A) $HgCl_2$	1) Tetrahedral
B) NH_4^+	2) Trigonal bipyramidal
C) SF_6	3) Linear
D) PCl_5	4) Octahedral

	A	B	C	D
a)	4	3	2	1
b)	3	1	4	2
c)	3	2	1	4
d)	2	3	4	1

Ans: (b)

Q.28. Which of the following statements is incorrect?

a) a double bond is stronger than a single bond b) a double bond is shorter than a single bond c) π bond is a weak bond d) π bond does not affect the shape of the molecule

Ans: (c) π bond is a weak bond

Q.29. How many σ and π bonds are present in C_2H_4?

a) 5 and 2 b) 5 and 1 c) 4 and 3 d) 4 and 1

Ans: (b) 5 and 1 (5σ bonds and 1π bond)

Q.30. In a NO_3^- ion, the number of lone pair and bond pairs of electrons on nitrogen are

a) 4,0 b) 0,4 c) 2,3 d) 0,5

Ans: (b) 0,4 (HNO_3 nitrogen is surrounded by one coordinate bond O, one double bond O, and one single bond –O-H)

Q.31.Which of the following pairs has an identical bond order?

a) CN^- and O_2^- b) O_2^- and CN^+ c) CN^+ and CN^- d) CN^- and NO^+

Ans: (d) CN^- and NO^+ (both have 14 electrons, BO = 3)

Q.32. Which of the following angle corresponds to sp^3 hybridization?

a) 180° b) 120° c) 109°28` d) 90°

Ans: (c) 109°28`

Q.33. Which of the following is not linear?

a) HF b) H_2S c) H_2 d) HI

Ans: (b) H_2S (bent or angular shape, sp^3, LP =2, BP = 2)

Q.34. The hybridization of P in PCl_5 is

a) sp^3 b) sp^3d c) sp^3d^2 d) sp^2

Ans: (b) sp^3d (LP=0, BP = 5)

Q.35. Which one of the following has a regular tetrahedral structure?

a) XeF_4 b) SF_4 c) BF_4^- d) $[Ni(CN)_4]^{2-}$

Ans: (c) BF_4^- (BP = 4 & LP = 0)

Q.36. Arrange the following molecules in order of increasing fundamental vibrational frequencies (NET 2018)

a) $O_2^{2-} < O_2^- < O_2 < O_2^+$ b) $O_2 < O_2^+ < O_2^- < O_2^{2-}$ c) $O_2^{2-} < O_2^- < O_2^+ < O_2$ d) $O_2^+ < O_2 < O_2^- < O_2^{2-}$

Ans: (a) $O_2^{2-} < O_2^- < O_2 < O_2^+$ (BO order is $1 < 1.5 < 2 < 2.5$; BO $\propto$ vibrational frequencies)

It can be expected that these time efficient innovative mnemonics will help students, scholars, and educators in chemical education at undergraduate, senior undergraduate, and postgraduate level to predict the bond order of homo and heteronuclear molecules and ions and their related properties without drawing electronic configuration of diatomic species using MOT. Experiments, *in vitro*, on 100 students, showed that, by using these innovative formulae, students could save up to 10–15 minutes in the examination hall when solving different problems on bond order and its related properties in inorganic chemistry. On the basis of this, I can strongly recommend using these time efficient innovative mnemonics in inorganic chemistry.

CHAPTER 5

INNOVATIVE MNEMONICS FOR THE PREDICTION OF THE BOND ORDER OF OXIDE BASED ACID RADICALS

In Chapter 4, formulae based mnemonics were discussed in a time efficient manner to predict the bond order of homo and heteronuclear diatomic species without basing the electronic configurations on molecular orbital theory (MOT).

In this chapter, methods to predict the bond order of oxide-based acid radicals will be discussed without revealing their Lewis structures in a time consuming manner. This chapter explores the results of this method and provides suggestions for context-based teaching, learning, and assessment. Previously, conventional methods have been used to predict the bond order of oxide-based acid radicals. Now, with the help of time efficient and innovative mnemonics, the bond order can be predicted using a simple molecular formula based on oxide-based acid radicals without focusing on their Lewis structures.

METHODOLOGY

A. The conventional method to predict the bond order of oxide-based acid radicals.

Remember the following steps to determine the bond order of an oxide-based acid radical:

- Draw the Lewis structure of the oxide-based acid radical;
- Count the total number of bonds;
- Count the number of bond groups between individual atoms;
- Divide the number of bonds between atoms by the total number of bond groups in the molecule to find the bond order of the oxide-based acid radical.

B. Innovative mnemonics to predict the bond order of an oxide-based acid radical.

The bond order of an oxide-based acid radical can be calculated using this simple molecular formulae in the following way:[9, 10]

Bond order (B. O.) = valency of the peripheral atom + (charge on acid radical/total number of peripheral atoms) = $V_o + (e/Np)$ = 2 + (charge on acid radical/total number of peripheral atoms)

V_o = valency of the oxygen atom = 2, e = charge on acid radical and Np = total number of peripheral atoms

RESULTS AND DISCUSSION

Methods to predict the bond order of oxide-based acid radicals using innovative mnemonics are provided below:

ClO_4^-: (valency of one peripheral atom oxygen = 2, charge on acid radical = -1, total number of peripheral atoms = 04), therefore B. O. = 2 + (-1/4) = 1.75

ClO_3^-: (valency of one peripheral atom oxygen = 2, charge on acid radical = -1, total number of peripheral atoms = 03), therefore B. O. = 2 + (-1/3) = 1.66

ClO_2^-: (valency of one peripheral atom oxygen = 2, Charge on acid radical = -1, total number of peripheral atoms = 02), therefore B. O. = 2 + (-1/2) = 1.5

AsO_4^{3-}: (valency of one peripheral atom oxygen = 2, charge on acid radical = -3, total number of peripheral atoms = 04), therefore B. O. = 2 + (-3/4) = 1.25

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[9] A. Das, "Innovative Mnemonics In Chemical Education: Review Article", *African Journal of Chemical Education* 8 (July 2018): 144-189, https://www.ajol.info/index.php/ajce/article/view/176086.

[10] A. Das, "Innovative Mnemonics Make Chemical Education Time Economic: A Pedagogical Review Article", *World Journal of Chemical Education* 6 (Sept 2018): 154 174, doi:10.12691/wjce-6-4-2, http://pubs.sciepub.com/wjce/6/4/2/index.html.

AsO_3^{3-}: (valency of one peripheral atom oxygen = 2, charge on acid radical = -3, total number of peripheral atoms = 03), therefore B. O. = 2 + (-3/3) = 1.0

SO_4^{2-}: (valency of peripheral atom oxygen = 2, charge on acid radical = -2, number of peripheral atoms = 04), therefore B. O. = 2 + (-2/4) = 1.5

SO_3^{2-}: (valency of peripheral atom oxygen = 2, charge on acid radical = -2, number of peripheral atoms = 03), therefore B. O. = 2 + (-2/3) = 1.33

PO_4^{3-}: (valency of peripheral atom oxygen = 2, charge on acid radical = -3, number of peripheral atoms = 04), therefore B. O. = 2 + (-3/4) = 1.25

BO_3^{3-}: (valency of peripheral atom oxygen = 2, charge on acid radical = -3, number of peripheral atoms = 03), therefore B. O. = 2 + (-3/3) = 1

CO_3^{2-}: (valency of peripheral atom oxygen = 2, charge on acid radical = -2, number of peripheral atoms = 03), therefore B. O. = 2 + (-2/3) = 1.33

SiO_4^{4-}: (valency of peripheral atom oxygen = 2, charge on acid radical = -4, number of peripheral atoms = 04), therefore B. O. = 2 + (- 4/4) = 1

THE APPLICATION OF BOND ORDER IN CHEMICAL EDUCATION:

The relationship between different bond parameters (bond length, bond strength, bond energy, thermal stability, and reactivity) and the bond order:

B. O. $\propto$ 1/bond length or bond distance;
B. O. $\propto$ bond strength;
B. O. $\propto$ bond energy;
B. O. $\propto$ bond dissociation energy;
B. O. $\propto$ thermal stability;
B. O. $\propto$ 1/reactivity

The correlations of the literature values of the bond distances (Å) for some oxide-based acid radicals with their predicted bond order values are as follows:

Literature values of the Cl-O average bond lengths in ClO_4^-, ClO_3^-, and ClO_2^- are 1.50, 1.57, and 1.64 (Å) for their predicted bond orders values 1.75, 1.6 and 1.5, respectively.

As-O average bond lengths in AsO_4^{3-} and AsO_3^{3-} are 1.75 and 1.77 (Å) for their predicted bond order values 1.25 and 1.0, respectively, which suggests that when the bond order increases, the bond length decreases.

It may be expected that this time effective and innovative mnemonic will help students and educators in chemical education at undergraduate, senior undergraduate, and postgraduate level to predict the bond order of oxide-based acid radicals without spending unnecessary time drawing Lewis structures. Experiments *in vitro* on 100 students showed that, by using this innovative formula, they could save between 2–3 minutes in the examination hall when solving different problems connected to bond orders and its related properties (bond length, bond strength, bond dissociation energy, etc.). On the basis of this, I can strongly recommend using this time-efficient and innovative mnemonic in inorganic chemistry.

CHAPTER 6

INNOVATIVE MNEMONICS FOR THE PREDICTION OF THE MAGNETIC BEHAVIOUR OF DIATOMIC SPECIES WITHOUT MOLECULAR ORBITAL THEORY

In Chapter 4, formulae based mnemonics that predict the bond order of homo and heteronuclear diatomic species without drawing their electronic configurations using molecular orbital theory (MOT) were discussed. In Chapter 5, the prediction of the bond order of oxide-based acid radicals in a time efficient way without drawing Lewis structures was discussed. In this chapter, the magnetic properties of diatomic species that have a total number of electrons (1–20) will be predicted without drawing their electronic configuration by using molecular orbital theory. Here, three time efficient innovative mnemonics will be discussed. This will also include three formulae to predict the magnetic behavior of diatomic species without using MOT. Conventionally, magnetic properties of diatomic species have been predicted using molecular orbital theory by counting the number of unpaired electrons present in the bonding molecular orbitals (BMOs) or the anti-bonding molecular orbitals (ABMOs) of diatomic species. In an electronic configuration, if the diatomic species contains unpaired or paired electrons in its bonding molecular orbitals (BMOs) and anti-bonding molecular orbitals (ABMOs), then it will be paramagnetic or diamagnetic, respectively.

Friedrich Hund and Robert Mulliken first proposed molecular orbital theory in 1933.[11] The three formulae, allow the unpaired electrons (n) to be manipulated. By using the mod function and n values, students can

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[11] R S. Mulliken, *Spectroscopy, Molecular Orbitals, and Chemical Bonding Nobel Lectures Chemistry* (Amsterdam Elsevier Publishing Company: 1972), 1963 1970; George G. Hall, "The Lennard-Jones Paper of 1929 and the foundations of Molecular Orbital Theory", Advances *in Quantum Chemistry* 22 (1991): 1 6, doi:10.1016/S0065-3276(08)60361-5.

easily stumble upon the magnetic moment values in Bohr-Magneton (B.M.) using the formula: $\mu_s = \sqrt{n(n+2)}$ B.M., where B.M. = Bohr Magneton = unit of magnetic moment and n = number of unpaired electrons.[12]

METHODOLOGY

A. The conventional method to predict the magnetic properties of diatomic species using molecular orbital theory.

Increasing the energetic order of different molecular orbitals for electrons ≤ 14

$$\sigma_{1s} < \sigma^*_{1s} < \sigma_{2s} < \sigma^*_{2s} < \pi_{2Px} = \pi_{2py} < \sigma_{2pz} < \pi^*_{2px} = \pi^*_{2py} < \sigma^*_{2pz}$$

Increasing the energetic order of different molecular orbitals for electrons > 14

$$\sigma_{1s} < \sigma^*_{1s} < \sigma_{2s} < \sigma^*_{2s} < \sigma_{2pz} < \pi_{2Px} = \pi_{2py} < \pi^*_{2px} = \pi^*_{2py} < \sigma^*_{2pz}$$

In this energetic order, there are five bonding molecular orbitals (BMOs)—σ_{1s}, σ_{2s}, π_{2px}, π_{2py}, σ_{2pz}—and five anti bonding molecular orbitals (ABMOs)—σ^*_{1s}, σ^*_{2s}, π^*_{2px}, π^*_{2py}, σ^*_{2pz}. The magnetic properties of diatomic species can be predicted from the electronic configuration of the diatomic species by counting the number of unpaired electrons present in their bonding molecular orbitals (BMOs) or anti-bonding molecular orbitals (ABMOs). If the diatomic species contains unpaired or paired electrons in its bonding molecular orbitals (BMOs) or anti-bonding

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[12] A. Das, "Bond Order and Magnetic Behavior of Diatomic Species without Molecular Orbital Theory", *World Journal of Chemical Education* 5 (June 2017): 128 131, doi: 10.12691/wjce-5-4-2, http://pubs.sciepub.com/wjce/5/4/2/; A. Das, "A Review of Time Economic Innovative Mnemonics In Chemical Education". *International Journal of Physics & Chemistry Education* 10 (June 2018): 27 40, doi: 10.12973/ijpce/81589, http://www.ijpce.org/A-Review-of-Time-Economic-Innovative-Mnemonics-in-Chemical-Education,81589,0,2.html; A. Das, "Innovative Mnemonics In Chemical Education: Review Article", *African Journal of Chemical Education* 8 (July 2018): 144 189, https://www.ajol.info/index.php/ajce/article/view/176086; A. Das, "Innovative Mnemonics Make Chemical Education Time Economic: A Pedagogical Review Article", *World Journal of Chemical Education* 6 (Sept 2018):154 174, doi:10.12691/wjce-6-4-2, http://pubs.sciepub.com/wjce/6/4/2/index.html.

molecular orbitals (ABMOs), then it will be paramagnetic or diamagnetic, respectively.

B. Innovative mnemonics to predict the magnetic properties of diatomic species without using molecular orbital theory.

First, classify the molecules or ions in three sets based on the total number of electrons present:

Set-1: Molecules or ions with (1–3)e^-s, (3–5)e^-s, (5–7)e^-s, (7–10)e^-s, or (13–16)e^-s

Set-2: Molecules or ions with (10–13)e^-s or (16–19)e^-s

Set-3: Molecules or ions with 20e^-s

Then for a different set, we have to use three different formulae to calculate the number of unpaired electrons. The magnetic moment (μ_s) in B.M. can be evaluated in the following way:

i) F-1 (for Set-1) to determine the number of unpaired electrons (n) in molecules or ions with (1–3), (3–5), (5–7), (7–10) and (13–16)e^-s:

In this case, the number of unpaired electrons is n = [I (ND - total e^-s) I], where ND = next digit (digit next to minimum digit) and II indicates the mod function.

Example: Molecules or ions with (1–3)e^-s; in this case, ND = 2 because the minimum digit is 1.

For molecules or ions containing (3–5)e^-s, (5–7)e^-s, (7–10)e^-s, and (13–16)e^-s, the ND value will be 4, 6, 8, and 14, respectively. Therefore, the value of n = [I (4-total e^-s) I], [I (6- total e^-s) I] [I (8- total e^-s) I] and [I (14- total e^-s) I], respectively.

ii) F-2 (for Set-2) to determine the number of unpaired electrons (n) in molecules or ions with (10–13) and (16–19) electrons:

The number of unpaired electrons n = [(PD - total e^-s) I], where, PD = penultimate digit.

For the molecules or ions containing (10–13) and (16–19)e^-s, the PD value will be 12 and 18, respectively. Therefore, the value of n = [I (12 - total e^-s) I] and [I (18 - total e^-s) I], respectively.

iii) F-3 (for Set-3) to determine the number of unpaired electrons (n) in molecules or ions with 20 electrons:

In this case, the number of unpaired electrons is $n = [(20 - \text{total } e^{-}\text{s})]$.

RESULTS AND DISCUSSION

A. Predicting magnetic properties using the conventional method of M.O.T.:

When using the conventional method, the magnetic properties of molecules or ions should be predicted in the following way:

Example: H_2 (number of electrons < 14): electronic configuration (E.C.) with M.O.T. σ_{1s}^2, unpaired electrons (n) = 0, diamagnetic in nature; H_2^+: E.C. is σ_{1s}^1, unpaired electrons (n) = 1, paramagnetic in nature; H_2^-: E.C. is $\sigma_{1s}^2, \sigma^*_{1s}{}^1$, unpaired electrons (n) = 1, paramagnetic in nature.

He_2: E.C. is $\sigma_{1s}^2, \sigma^*_{1s}{}^2$, unpaired electrons (n) = 0, diamagnetic in nature; **He_2^+:** E.C. is $\sigma_{1s}^2, \sigma^*_{1s}{}^1$, unpaired electrons (n) = 1, paramagnetic in nature.

Li_2: E.C. is σ_{1s}^2, $\sigma^*_{1s}{}^2$, σ_{2s}^2, unpaired electrons (n) = 0, diamagnetic in nature; **Be_2:** E.C. is σ_{1s}^2, $\sigma^*_{1s}{}^2$, σ_{2s}^2, $\sigma^*_{2s}{}^2$, unpaired electrons (n) = 0, diamagnetic in nature; **B_2:** E.C. is σ_{1s}^2, $\sigma^*_{1s}{}^2$, σ_{2s}^2, $\sigma^*_{2s}{}^2$, π_{2px}^1, π_{2py}^1 (Fig. 4.22), unpaired electrons (n) = 2, paramagnetic in nature; **C_2:** E.C. is σ_{1s}^2, $\sigma^*_{1s}{}^2$, σ_{2s}^2, $\sigma^*_{2s}{}^2$, π_{2px}^2, π_{2py}^2, unpaired electrons (n) = 0, diamagnetic in nature.

N_2: E.C. is σ_{1s}^2, $\sigma^*_{1s}{}^2$, σ_{2s}^2, $\sigma^*_{2s}{}^2$, π_{2px}^2, π_{2py}^2, σ_{2pz}^2, unpaired electrons (n) = 0, diamagnetic in nature; **N_2^+:** E.C. is σ_{1s}^2, $\sigma^*_{1s}{}^2$, σ_{2s}^2, $\sigma^*_{2s}{}^2$, π_{2px}^2, π_{2py}^2, σ_{2pz}^1, unpaired electrons (n) = 1, paramagnetic in nature; **N_2^- :** E.C. is σ_{1s}^2, $\sigma^*_{1s}{}^2$, σ_{2s}^2, $\sigma^*_{2s}{}^2$, π_{2px}^2, π_{2py}^2, σ_{2pz}^2 , $\pi^*_{2px}{}^1$, unpaired electrons (n) = 1, paramagnetic in nature; **N_2^{2-} :** E.C. is σ_{1s}^2, $\sigma^*_{1s}{}^2$, σ_{2s}^2, $\sigma^*_{2s}{}^2$, π_{2px}^2, π_{2py}^2, σ_{2pz}^2 , $\pi^*_{2px}{}^1$, $\pi^*_{2py}{}^1$, unpaired electrons (n) = 2, paramagnetic in nature.

O_2 (number of electrons > 14): E.C. of O_2 is σ_{1s}^2, $\sigma^*_{1s}{}^2$, σ_{2s}^2, $\sigma^*_{2s}{}^2$, σ_{2pz}^2, π_{2px}^2, π_{2py}^2, $\pi^*_{2px}{}^1$, $\pi^*_{2py}{}^1$ (Fig. 4.23), unpaired electrons (n) = 2, paramagnetic in nature; **O_2^+:** E.C. is σ_{1s}^2, $\sigma^*_{1s}{}^2$, σ_{2s}^2, $\sigma^*_{2s}{}^2$, σ_{2pz}^2, π_{2px}^2, π_{2py}^2, $\pi^*_{2px}{}^1$, unpaired electrons (n) = 1, paramagnetic in nature; **O_2^-:** E.C. is σ_{1s}^2, $\sigma^*_{1s}{}^2$, σ_{2s}^2, $\sigma^*_{2s}{}^2$, σ_{2pz}^2, π_{2px}^2, π_{2py}^2, $\pi^*_{2px}{}^2$, $\pi^*_{2py}{}^1$, unpaired electrons (n) = 1, paramagnetic in nature; **O_2^{2-}:** E.C. is σ_{1s}^2, $\sigma^*_{1s}{}^2$, σ_{2s}^2, $\sigma^*_{2s}{}^2$, σ_{2pz}^2, π_{2px}^2, π_{2py}^2, $\pi^*_{2px}{}^2$, $\pi^*_{2py}{}^2$, unpaired electrons (n) = 0, diamagnetic in nature.

F_2: E.C. is σ_{1s}^2, $\sigma^*_{1s}{}^2$, σ_{2s}^2, $\sigma^*_{2s}{}^2$, σ_{2pz}^2, π_{2px}^2, π_{2py}^2, $\pi^*_{2px}{}^2$, $\pi^*_{2py}{}^2$, unpaired electrons (n) = 0, diamagnetic in nature.

Ne_2: E.C. is σ_{1s}^2, $\sigma^*_{1s}{}^2$, σ_{2s}^2, $\sigma^*_{2s}{}^2$, σ_{2pz}^2, π_{2px}^2, π_{2py}^2, $\pi^*_{2px}{}^2$, $\pi^*_{2py}{}^2$, $\sigma^*_{2pz}{}^2$, unpaired electrons (n) = 0, diamagnetic in nature.

CN (number of electrons < 14): E.C. is σ_{1s}^2, $\sigma^*_{1s}{}^2$, σ_{2s}^2, $\sigma^*_{2s}{}^2$, π_{2px}^2, π_{2pv}^2, σ_{2pz}^1, unpaired electrons (n) = 1, paramagnetic in nature; **CN^-:** E.C. is σ_{1s}^2, $\sigma^*_{1s}{}^2$, σ_{2s}^2, $\sigma^*_{2s}{}^2$, π_{2px}^2, π_{2py}^2, σ_{2pz}^2, unpaired electrons (n) = 0, diamagnetic in nature.

NO (number of electrons > 14): E.C. is σ_{1s}^2, $\sigma^*_{1s}{}^2$, σ_{2s}^2, $\sigma^*_{2s}{}^2$, σ_{2pz}^2, π_{2px}^2, π_{2py}^2, $\pi^*_{2px}{}^1$, unpaired electrons (n) = 1, paramagnetic in nature; **NO^+:** E.C. is σ_{1s}^2, $\sigma^*_{1s}{}^2$, σ_{2s}^2, $\sigma^*_{2s}{}^2$, σ_{2pz}^2, π_{2px}^2, π_{2py}^2, unpaired electrons (n) = 0, diamagnetic in nature.

B. Predicting magnetic properties using innovative mnemonics without M.O.T.:

The present study involves three new formulae that manipulate the number of unpaired electrons (n) using the mod function (which is based on Applied Mathematics). From these "n" values, the magnetic moment values in Bohr-Magneton can be calculated using a spin formula: $\mu_s = \sqrt{n(n+2)}$ B.M., where B.M. = Bohr Magneton = unit of magnetic moment; n = number of unpaired electrons.

First, classify the molecules or ions depending on the total number of electrons present in the following three (03) sets:

Set-1: Molecules or ions with (1–3)e-s, (3–5)e-s, (5–7)e-s, (7–10)e-s, (13–16)e-s

Set-2: Molecules or ions with (10–13)e-s and (16–19)e-s

Set-3: Molecules or ions with 20e-s

Three different formulae are used to calculate the number of unpaired electrons (n) in the different sets (see Table 5.5). The magnetic moment values (μ_s), in B.M. can be evaluated from the number of unpaired electrons (n) in the following way:

F-1 (for Set-1) to determine the number of unpaired electrons (n) of molecules or ions with (1–3), (3–5), (5–7), (7–10), and (13–16)e-s.

In this case, the number of unpaired electrons is n = [I (ND - total e-s) I], where, ND = next digit (i.e. the digit next to minimum digit) and “II” indicates the mod function. For molecules or ions with (1–3)e-s, ND = 2 because the minimum digit is 1.

Example A: In He_2^+ (3e-s), the total number of electrons will be 3, ND = 2. Therefore, the unpaired electrons is n = I (ND - total e-s) I = I (2-3) I = 1 and the magnetic moment is $\mu_s = \sqrt{n(n+2)}$ B.M. = $\sqrt{1(1+2)}$ BM = $\sqrt{3}$ BM = 1.73 B.M.

For molecules or ions containing (3–5)e-s, (5–7)e-s, (7–10)e-s, and (13–16)e-s, the ND value will be 4, 6, 8, and 14, respectively. Hence, the value of n = [I (4-total e-s) I], [I (6- total e-s)I] [I (8- total e-s) I], and [I (14-total e-s) I], respectively.

F-2 (for Set-2) to determine the number of unpaired electrons (n) in molecules or ions with (10–13) and (16–19) electrons:

In this case, the number of unpaired electrons n = [I (PD - total e-s) I], where PD = penultimate digit.

Example B: In C_2^- (13e-s), the total number of electrons will be 13, PD = 12. Hence, the unpaired electrons is n = I (12 - total e-s) I = I (12-13) I = 1 and the magnetic moment is $\mu_s = \sqrt{n(n+2)}$ B.M. = $\sqrt{1(1+2)}$ B.M. = $\sqrt{3}$ B.M. = 1.73 B.M.

Example C: In F_2 (18e-s), the total number of electrons will be 18, PD = 18. Hence, the unpaired electrons is n = I (18 - total e^-s) I = I (18-18) I = 0 and the magnetic moment is $\mu_s = \sqrt{n(n+2)}$ B.M. = $\sqrt{0(0+2)}$ B.M. = 0 B.M.= diamagnetic in nature.

F-3 (for Set-3) in order to determine the number of unpaired electrons (n) in molecules or ions with 20 electrons.

In this case, the number of unpaired electrons is n = [I (20 - total e-s)I].

Example D: In Ne_2 (20e-s), the total number of electrons will be 20; hence, the unpaired electrons is n = I (20 - total e-s) I = I (20-20) I = 0, and the magnetic moment is $\mu_s = \sqrt{n(n+2)}$ B.M. = $\sqrt{0(0+2)}$ B.M. = 0 B.M. = diamagnetic in nature.

MAGNETIC PROPERTIES PROBLEMS

(Using Magnetic Properties Mnemonics to Solve Problems in Competitive Exams)

Q.1. Which of the following species is not paramagnetic? (JEE MAIN 2017)

a) NO b) CO c) O_2 d) B_2

Ans: (b)

Q.2. Which molecules exhibit diamagnetic behaviour?

a) C_2 b) N_2 c) O_2 d) S_2 (JEE MAIN 2013)

Ans: (a), (b)

Q.3. Which of the following is paramagnetic? (NEET 2013)

a.) CO b) O_2^- c) CN^- d) NO^+

Ans: (b)

[Total e-s = 16+1 = 17, unpaired e^-s n = [I (PD - total e^-s)I] = [I (18 - 17)I] = 1, because it belongs to SET 2: (16-19) e^-s, where PD = penultimate digit = 18]

Q.4. Which of the following species is diamagnetic?

a) B_2 b) N_2^+ c) N_2^- d) N_2^{2+}

Ans: (d) Total electrons 12, n = 0, magnetic moment, $\mu_s = 0$ B.M.

Q.5. The number of unpaired electrons in a CO molecule is

a) 0 b) 1 c) 2 d) 3

Ans: (a)

Q.6. Which of the following species is paramagnetic? (CBSE AIPMT 1995)

a) O_2^{2-} b) NO c) CO d) CN^-

Ans: (b)

Q.7. Which of the following is not paramagnetic?

a) NO b) F_2 c) O_2^- d) N_2^-

Ans: (b), all electrons in BMOs and ABMOs are paired

Q.8. Paramagnetism is exhibited by molecules which

a) are not attracted by magnetic field b) contain only paired electrons c) contain unpaired electrons d) carry positive charge.

Ans: (b)

Q.9. Which of the following species is paramagnetic?

a) CO_2 b) NO c) O_2^{2-} d) CN^-

Ans: (b), contains an unpaired electrons in ABMO $\pi^*{}_{2px}^{1}$

Q.10. An O_2 molecule is

a) paramagnetic b) diamagnetic c) ferromagnetic d) none of these

Ans: (a)

Q.11. The molecule with one unpaired electrons is

a) NO b) CO_2 c) CN^- d) O_2

Ans: (a), there is one unpaired electrons in ABMO, $\pi^*{}_{2px}$ (E.C. of NO is $\sigma_{1s}{}^2$, $\sigma^*{}_{1s}{}^2$, $\sigma_{2s}{}^2$, $\sigma^*{}_{2s}{}^2$, $\sigma_{2pz}{}^2$, $\pi_{2Px}{}^2$, $\pi_{2py}{}^2$, $\pi^*{}_{2px}{}^1$)

Q.12. Which of the following species is paramagnetic?

a) O_2^- b) CN^- c) CO d) NO^+

Ans: (a), E.C. of O_2^- is $\sigma_{1s}{}^2$, $\sigma^*{}_{1s}{}^2$, $\sigma_{2s}{}^2$, $\sigma^*{}_{2s}{}^2$, $\sigma_{2pz}{}^2$, $\pi_{2Px}{}^2$, $\pi_{2py}{}^2$, $\pi^*{}_{2px}{}^2$, $\pi^*{}_{2py}{}^1$

Q.13. Which of the following molecular species has an unpaired electron(s)?

a) N_2 b) F_2 c) O_2^- d) O_2^{2-}

Ans: (c), E.C. of O_2^- is $\sigma_{1s}{}^2$, $\sigma^*{}_{1s}{}^2$, $\sigma_{2s}{}^2$, $\sigma^*{}_{2s}{}^2$, $\sigma_{2pz}{}^2$, $\pi_{2Px}{}^2$, $\pi_{2py}{}^2$, $\pi^*{}_{2px}{}^2$, $\pi^*{}_{2py}{}^1$

Q.14. According to molecular orbital theory, which of the following statements about the magnetic character and bond order is correct with regard to O_2^+?

a) paramagnetic and bond order < O_2 b) paramagnetic and bond order > O_2
c) diamagnetic and bond order < O_2 d) diamagnetic and bond order > O_2

Ans: (b)

Q.15. Which molecule contains an odd electron (STGT 2017)?

a) O_2 b) NO c) CO d) H_2S

Ans: (b), in NO, the total number of electrons = 15 and so it belongs to set 1: (13–16)e^-s, where ND = 14. Therefore, the number of unpaired electrons are n = I(ND - total e^-s)I = I14-15I = 1] (see Table 5.5)

It can be expected that these time efficient innovative mnemonics that predict magnetic properties without molecular orbital theory will be helpful for both students and educators in inorganic chemical education at undergraduate, senior undergraduate, and postgraduate level. This will allow students to predict the magnetic moments of homo and heteronuclear molecules and ions without drawing the electronic configuration of the diatomic species. Experiments, *in vitro*, on 100 students showed that, by using these innovative formulae, students could save up to 10–15 minutes in the examination hall when solving different problems related to magnetic properties. On the basis of this, I can strongly recommend using these time efficient innovative mnemonics in inorganic chemistry.

CHAPTER 7

INNOVATIVE MNEMONICS FOR THE PREDICTION OF SPIN MULTIPLICITY

Chapter 6 discussed formulae based mnemonics that can be used to predict the magnetic properties of diatomic species with between 1 and 20 electrons without using molecular orbital theory (MOT) to draw their electronic configurations. In this chapter, the spin multiplicity values have been predicted by other innovative mnemonics without calculating the total spin quantum numbers (S) of elements, molecules, or ions, and coordination compounds. The spin multiplicity is integral to finding the atomic symbol, ${}^{2S+1}L_J$, along with resultant vectors L and J in co-ordination chemistry.[13] L is also known as a resultant orbital angular momentum quantum number.

Friedrich Hund first discovered the spin multiplicity value and its corresponding spin state in 1925. The formula that is generally used to predict the spin multiplicity value is (2S+1), where $S = \Sigma s$ = total spin quantum number. This method is time-consuming.[14] Therefore, we have created simple innovative mnemonics to calculate the spin-multiplicity value and its corresponding spin state. This method ignores the total spin quantum number ($S = \Sigma s$).

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[13] J. E. Huheey, *et.al. Inorganic Chemistry* (Pearson, 4th ed., India: 2006), 711 715.

[14] T. Engel and P. Reid*Physical Chemistry* (Pearson Benjamin-Cunmings: 2006), 473, 477 479.

METHODOLOGY

A. The conventional method to predict the spin multiplicity of elements and compounds

$(2S+1)$, where $S = \Sigma s$ = total spin quantum number.

B. Innovative mnemonics to predict the spin multiplicity of elements and compounds

First of all, classify the unpaired electrons of species (atoms, molecules, ions, or complexes) and then the spin

multiplicity value should be evaluated into three types based upon the nature of their alignment.[15]

i) Species with unpaired electrons in an upward alignment (↑)

Spin multiplicity = $(n+1)$; where n = number of unpaired electrons

ii) Species with unpaired electrons in a downward alignment (↓):

Spin multiplicity = $(-n+1)$, where the -ve sign indicates a downward arrow.

iii) Species with unpaired electrons in mixed alignments (↑) (↓):

Spin multiplicity = $[(+n) + (-n) + 1]$, where n = number of unpaired electrons. Here, the +ve and –ve signs indicate the electrons' upward or downward alignment, respectively.

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RESULTS AND DISCUSSION

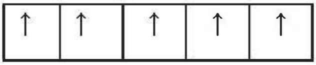
A. Predicting the spin multiplicity of elements, molecules, and compounds using the conventional method

The formula that is generally used to predict the spin multiplicity value is 2S+1, where S = Σs = total spin quantum number.

First of all, draw the electronic configurations using the Aufbau principle, MOT, and CFT (crystal field theory) and then calculate the total spin quantum number (S) to find the unpaired electrons. After this is done, then evaluate the spin multiplicity value by putting the value of "S" in 2S+1 to find the corresponding spin state.

Example A: Predicting the spin multiplicity value for manganese Mn (Z = 25)

The electronic configuration of Mn, using the Aufbau principle, is $1s^2$, $2s^2$, $2p^6$, $3s^2$, $3p^6$, $4s^2$, $3d^5$



($3d^5$ electronic distribution in five d orbitals)

Here, s = +1/2 +1/2 +1/2 +1/2 +1/2, s = spin quantum number, which is (+1/2) and (-1/2) for the upward alignment of the electrons. Here, S = Σs = total spin quantum number = (+5/2). The spin multiplicity value = 2S + 1 = 2 (+5/2) + 1 = 6 (spin state: sextet).

Example B: Predicting the spin multiplicity value for the oxygen molecule, O_2 (16e⁻s)

Using MOT, the electronic configuration of O_2 with 16 electrons is $\sigma_{1s}{}^2$, $\sigma^*{}_{1s}{}^2$, $\sigma_{2s}{}^2$, $\sigma^*{}_{2s}{}^2$, $\sigma_{2pz}{}^2$, $\pi_{2px}{}^2$, $\pi_{2py}{}^2$, $\pi^*{}_{2px}{}^1$, and $\pi^*{}_{2py}{}^1$ (Fig. 4.23). From this electronic configuration, it is clear that there are 2 unpaired electrons in 2 anti-bonding molecular orbitals ($\pi^*{}_{2px}$, $\pi^*{}_{2py}$), where S = Σs = total spin quantum number = (+1/2) + (1/2) = 1. This means that the spin multiplicity value = 2S + 1 = 2 (1) + 1 = 3 (spin state: triplet).

Example C: Predicting the spin multiplicity value for molecular ion O_2^+ (15e⁻s)

Using MOT, the electronic configuration of O_2^+ with 15 electrons is $\sigma_{1s}{}^2$, $\sigma^*{}_{1s}{}^2$, $\sigma_{2s}{}^2$, $\sigma^*{}_{2s}{}^2$, $\sigma_{2pz}{}^2$, $\pi_{2px}{}^2$, $\pi_{2py}{}^2$, $\pi^*{}_{2px}{}^1$, and $\pi^*{}_{2py}{}^0$. From this electronic configuration, it is clear that there is 1 unpaired electron in 1 anti-bonding molecular orbital (π^*_{2px}), where $S = \Sigma s$ = total spin quantum number = +1/2. This means that the spin multiplicity value = $2S + 1 = 2 (+1/2) + 1 = 2$ (spin state: doublet).

Example D: Predicting the spin multiplicity value for a high spin Mn^{2+} octahedral complex ($3d^5$). Using crystal field theory (CFT), the electronic configuration for a high spin Mn^{2+} octahedral complex ($3d^5$) is t_{2g}^3, e_g^2, where the number of unpaired electrons in an upward alignment are n = 5. Here, $S = \Sigma s$ = total spin quantum number = +5/2. This means that the spin multiplicity value = $2S + 1 = 2 (+5/2) + 1 = 6$ (spin state: sextet).

B. Predicting the spin multiplicity of elements, molecules, and compounds using innovative mnemonics

First of all, classify the species (atoms, molecules, ions, or complexes), where the spin multiplicity value and its corresponding spin state are based on three types depending on the nature of the alignment of the unpaired electrons (upward, downward, or mixed).

i) *Upward alignment*

Spin multiplicity = (n +1), where n = number of unpaired electrons.

Example

↑		
↑	↑	
↑	↑	↑

The spin multiplicity = (n +1) = (1+1) = 2 (spin state = doublet); (2+1) = 3 (spin state = triplet); and (3 + 1) = 4 (spin state = quartet), respectively.

↑↓	↑	↑
↑↓	↑↓	↑

The spin multiplicity = (n +1) = (2 + 1) = 3 (in this case ignore paired electrons) (spin state = triplet) and (1 + 1) = 2 (spin state = doublet).

↑↓	↑↓	↑↓

Spin multiplicity = (n +1) = (0 + 1) = 1 (spin state = singlet).

ii) *Downward alignment*

Spin multiplicity = (-n +1), where, n = number of unpaired electrons.

Example

↓		
↓	↓	
↓	↓	↓

Spin multiplicity = (-1 + 1) = 0; (-2 + 1) = -1 and (-3 + 1) = -2.

↑↓	↓	↓
↑↓	↑↓	↓

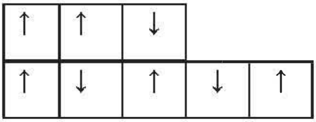
Spin multiplicity = (-n + 1) = (-2 + 1) = -1 (ignore paired electrons) and (-1 + 1) = 0.

iii) *mixed (upward and downward) alignment (a completely hypothetical assumption)*

Spin multiplicity = [(+n) + (-n) +1], where (+n) = upward directed unpaired electron and (-n) = downward directed unpaired electron.

Example

↑	↓	



Spin multiplicity = [(+n) + (-n) +1] = [(+1) + (-1) + 1] = 1 (spin state = singlet); [(+2) + (-1) + 1] = 2 (spin state = doublet) and [(+3) + (-2) +1] = 2 (spin state = doublet).

For 1, 2, 3, 4, 5, 6 or > 6 spin multiplicity values (n+1), the corresponding spin state will be a singlet, doublet, triplet, quartet, quintet, sextet, or multiplet, respectively.

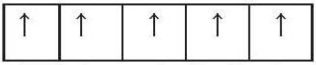
USING MNEMONICS TO PREDICT THE SPIN MULTIPLICITY VALUE OF ELEMENTS, MOLECULES, IONS, AND CO-ORDINATION COMPOUNDS

First of all, draw the electronic configurations using the Aufbau principle, MOT and CFT, respectively. After this, calculate the number of unpaired electrons (n) and then evaluate the spin multiplicity value by putting the value of “n” in the innovative formulae. This will provide the corresponding spin state.

Predicting the spin multiplicity of an element:

Example Predict the spin multiplicity value for manganese Mn (Z = 25) by drawing an electronic configuration using the Aufbau principle and Hund's rule.

The electronic configuration of Mn using the Aufbau principle is $1s^2$, $2s^2$, $2p^6$, $3s^2$, $3p^6$, $4s^2$, $3d^5$



($3d^5$ electronic distribution in five d orbitals)

Here, n = number of unpaired electrons = 5. The spin multiplicity value = (n + 1) = (n + 1) = 5 + 1 = 6 (spin state: sextet).

Predicting the spin multiplicity of a molecule:

Example Predict the spin multiplicity value for an oxygen molecule O_2 (16e^-s) by drawing an electronic configuration using MOT.

Using MOT, the electronic configuration of O_2 with16 electrons is $\sigma_{1s}{}^2$, $\sigma^*_{1s}{}^2$, $\sigma_{2s}{}^2$, $\sigma^*_{2s}{}^2$, $\sigma_{2pz}{}^2$, $\pi_{2px}{}^2$, $\pi_{2py}{}^2$, $\pi^*_{2px}{}^1$, $\pi^*_{2py}{}^1$ (Fig. 4.23). From this electronic configuration, n = number of unpaired electrons = 2. This means the spin multiplicity value = (n + 1) = 2 + 1 = 3 (spin state: triplet).

Predicting the spin multiplicity of a molecular ion

Example Predicting the spin multiplicity value for molecular ion O_2^+ (15e$^-$s) by drawing the electronic configuration using MOT.

Using MOT, the electronic configuration of O_2^+ with 15 electrons is $\sigma_{1s}{}^2$, $\sigma^*_{1s}{}^2$, $\sigma_{2s}{}^2$, $\sigma^*_{2s}{}^2$, $\sigma_{2pz}{}^2$, $\pi_{2px}{}^2$, $\pi_{2py}{}^2$, $\pi^*_{2px}{}^1$, $\pi^*_{2py}{}^0$. From this electronic configuration, n = number of unpaired electrons = 1. This means the spin multiplicity value = (n + 1) = 1 + 1 = 2 (spin state: doublet).

Predicting the spin multiplicity of high spin and low spin coordination compounds:

Example A: Predicting the spin multiplicity value for high spin and low spin octahedral complexes (coordination no 6) from first-row transition series elements ($3d^1$ to $3d^{10}$).

As per CFT, the five degenerate (same energy) d orbitals from octahedral complexes with a ligand field (LF) split into two set, t_{2g} and e_g. Three d orbitals (dxy, dyz, dxz) form a t_{2g} set and the other two (d_{x2-y2}, $d_z{}^2$) form an e_g set. In octahedral splitting, a t_{2g} set will be lower in energy than an e_g set. The energy difference between a t_{2g} and e_g set is to be treated according to the crystal field splitting energy of octahedral distortion and it is represented by Δ_o (Fig. 7.24).

The electronic configuration (EC) for low spin (LS) octahedral complexes with CFT and their corresponding spin multiplicity value and spin state can be calculated as follows:

For $3d^1$(LS), electronic representation – ($t_{2g}{}^1$, $e_g{}^0$), EC – ($t_{2g}{}^1$, $e_g{}^0$), number of unpaired electrons (n) = 1, spin multiplicity value (n+1) = (1+1) = 2. The spin state is doublet.

For $3d^2$(LS), electronic representation – ($t_{2g}{}^{1,\,2}$, $e_g{}^0$), EC - $t_{2g}{}^2$, $e_g{}^0$, number of unpaired electrons (n) = 2, spin multiplicity value (n+1) = (2+1) = 3. The spin state is triplet.

For 3d^3(LS), electronic representation – ($t_{2g}^{1,2,3}$, e_g^0), EC - t_{2g}^3, e_g^0, number of unpaired electrons (n) = 3, spin multiplicity value (n+1) = (3+1) = 4. The spin state is quartet.

For 3d^4(LS), electronic representation – ($t_{2g}^{1,2,3,4}$, e_g^0), EC - t_{2g}^4, e_g^0, number of unpaired electrons (n) = 2, spin multiplicity value (n+1) = (2+1) = 3. The spin state is triplet.

For 3d^5(LS), electronic representation – ($t_{2g}^{1,2,3,4,5}$, e_g^0), EC - t_{2g}^5, e_g^0, number of unpaired electrons (n) = 1, spin multiplicity value (n+1) = (1+1) = 2. The spin state is doublet.

For 3d^6(LS), electronic representation – ($t_{2g}^{1,2,3,4,5,6}$, e_g^0), EC - t_{2g}^6, e_g^0, number of unpaired electrons (n) = 0, spin multiplicity value (n+1) = (0+1) = 1. The spin state is singlet (lowest spin state).

For 3d^7(LS), electronic representation – ($t_{2g}^{1,2,3,4,5,6}$, e_g^7), EC - t_{2g}^6, e_g^1, number of unpaired electrons (n) = 1, spin multiplicity value (n+1) = (1+1) = 2. The spin state is doublet.

For 3d^8(LS), electronic representation – ($t_{2g}^{1,2,3,4,5,6}$, $e_g^{7,8}$), EC - t_{2g}^6, e_g^2, number of unpaired electrons (n) = 2, spin multiplicity value (n+1) = (2+1) = 3. The spin state is triplet.

For 3d^9(LS), electronic representation – ($t_{2g}^{1,2,3,4,5,6}$, $e_g^{7,8,9}$), EC - t_{2g}^6, e_g^3, number of unpaired electrons (n) = 1, spin multiplicity value (n+1) = (1+1) = 2. The spin state is doublet.

For 3d^{10}(LS), electronic representation – ($t_{2g}^{1,2,3,4,5,6}$, $e_g^{7,8,9,10}$), EC - t_{2g}^6, e_g^4, number of unpaired electrons (n) = 0, spin multiplicity value (n+1) = (0+1) = 1. The spin state is singlet (lowest spin state).

The electronic configuration (EC) for high spin (HS) octahedral complexes with CFT and their corresponding spin multiplicity value and spin state can be calculated as follows:

For 3d^1(HS), electronic representation – (t_{2g}^1, e_g^0), EC – (t_{2g}^1, e_g^0), number of unpaired electrons (n) = 1, spin multiplicity value (n+1) = (1+1) = 2. The spin state is doublet.

For 3d^2(HS), electronic representation – ($t_{2g}^{1,2}$, e_g^0), EC – (t_{2g}^2, e_g^0), number of unpaired electrons (n) = 2, spin multiplicity value (n+1) = (2+1) = 3. The spin state is triplet.

For 3d^3(HS), electronic representation – ($t_{2g}^{1,2,3}$, e_g^0), EC – (t_{2g}^3, e_g^0), number of unpaired electrons (n) = 3, spin multiplicity value (n+1) = (3+1) = 4. The spin state is quartet.

For 3d^4(HS), electronic representation – ($t_{2g}^{1,2,3}$, e_g^4), EC – (t_{2g}^3, e_g^1), number of unpaired electrons (n) = 4, spin multiplicity value (n+1) = (4+1) = 5. The spin state is quintet.

For 3d^5(HS), electronic representation – ($t_{2g}^{1,2,3}$, $e_g^{4,5}$), EC – (t_{2g}^3, e_g^2), number of unpaired electrons (n) = 5, spin multiplicity value (n+1) = (5+1) = 6. The spin state is sextet (highest spin state).

For 3d^6(HS), electronic representation – ($t_{2g}^{1,2,3}$, $e_g^{4,5}$, t_{2g}^6), EC – (t_{2g}^4, e_g^2), number of unpaired electrons (n) = 4, spin multiplicity value (n+1) = (4+1) = 5. The spin state is quintet.

For 3d^7(HS), electronic representation – ($t_{2g}^{1,2,3}$, $e_g^{4,5}$, $t_{2g}^{6,7}$), EC – (t_{2g}^5, e_g^2), number of unpaired electrons (n) = 3, spin multiplicity value (n+1) = (3+1) = 4. The spin state is quartet.

For 3d^8(HS), electronic representation – ($t_{2g}^{1,2,3}$, $e_g^{4,5}$, $t_{2g}^{6,7,8}$), EC – (t_{2g}^6, e_g^2), number of unpaired electrons (n) = 2, spin multiplicity value (n+1) = (2+1) = 3. The spin state is triplet.

For 3d^9(HS), electronic representation – ($t_{2g}^{1,2,3}$, $e_g^{4,5}$, $t_{2g}^{6,7,8}$, e_g^9), EC – (t_{2g}^6, e_g^3), number of unpaired electrons (n) = 1, spin multiplicity value (n+1) = (1+1) = 2. The spin state is doublet.

For 3d^{10}(HS), electronic representation – ($t_{2g}^{1,2,3}$, $e_g^{4,5}$, $t_{2g}^{6,7,8}$, $e_g^{9,10}$), EC – (t_{2g}^6, e_g^4), number of unpaired electrons (n) = 0, spin multiplicity value (n+1) = (0+1) = 1. The spin state is singlet (lowest spin state).

Example B: Predicting the spin multiplicity value for the high spin and low spin tetrahedral complexes (coordination no 4) of first-row transition series elements (3d^1 to 3d^{10}).

As per CFT, the five degenerate (same energy) d orbitals of tetra complexes in the presence of a ligand field (LF) will split into two sets, t_{2g} and e_g. Three d orbitals (dxy, dyz, dxz) form a t_{2g} set and the other two ($d_{x2\text{-}y2}$, d_z^2) form an e_g set. In tetrahedral splitting, a t_{2g} set will be higher in energy than an e_g set. The energy difference between an e_g and t_{2g} set should be treated using a crystal field splitting energy from a tetrahedral distortion and this is represented by Δ_t (Fig. 7.24).

The electronic configuration (EC) for high spin (HS) tetrahedral complexes with CFT and their corresponding spin multiplicity value and spin state can be calculated as follows:

For $3d^1$(HS), electronic representation – (e_g^1, t_{2g}^0), EC – (t_{2g}^0, e_g^1), number of unpaired electrons (n) = 1, spin multiplicity value (n+1) = (1+1) = 2. The spin state is doublet.

For $3d^2$(HS), electronic representation – ($e_g^{1,2}$, t_{2g}^0), EC – (t_{2g}^0, e_g^2), number of unpaired electrons (n) = 2, spin multiplicity value (n+1) = (2+1) = 3. The spin state is triplet.

For $3d^3$(HS), electronic representation – ($e_g^{1,2}$, t_{2g}^3), EC – (t_{2g}^1, e_g^2), number of unpaired electrons (n) = 3, spin multiplicity value (n+1) = (3+1) = 4. The spin state is quartet.

For $3d^4$(HS), electronic representation – ($e_g^{1,2}$, $t_{2g}^{3,4}$), EC – (t_{2g}^2, e_g^2), number of unpaired electrons (n) = 4, spin multiplicity value (n+1) = (4+1) = 5. The spin state is quintet.

For $3d^5$(HS), electronic representation – ($e_g^{1,2}$, $t_{2g}^{3,4,5}$), EC – (t_{2g}^3, e_g^2), number of unpaired electrons (n) = 5, spin multiplicity value (n+1) = (5+1) = 6. The spin state is sextet (highest spin state).

For $3d^6$(HS), electronic representation – ($e_g^{1,2}$, $t_{2g}^{3,4,5}$, e_g^6), EC – (t_{2g}^3, e_g^3), number of unpaired electrons (n) = 4, spin multiplicity value (n+1) = (4+1) = 5. The spin state is quintet.

For $3d^7$(HS), electronic representation – ($e_g^{1,2}$, $t_{2g}^{3,4,5}$, $e_g^{6,7}$), EC – (t_{2g}^3, e_g^4), number of unpaired electrons (n) = 3, spin multiplicity value (n+1) = (3+1) = 4. The spin state is quartet.

For $3d^8$(HS), electronic representation – ($e_g^{1,2}$, $t_{2g}^{3,4,5}$, $e_g^{6,7}$, t_{2g}^8), EC – (t_{2g}^4, e_g^4), number of unpaired electrons (n) = 2, spin multiplicity value (n+1) = (2+1) = 3. The spin state is triplet.

For $3d^9$(HS), electronic representation – ($e_g^{1,2}$, $t_{2g}^{3,4,5}$, $e_g^{6,7}$, $t_{2g}^{8,9}$), EC – (t_{2g}^5,e_g^4), number of unpaired electrons (n) = 1, spin multiplicity value (n+1) = (1+1) = 2. The spin state is doublet.

For $3d^{10}$(HS), electronic representation – ($e_g^{1,2}$, $t_{2g}^{3,4,5}$, $e_g^{6,7}$, $t_{2g}^{8,9,10}$), EC – (t_{2g}^6, e_g^4), number of unpaired electrons (n) = 0, spin multiplicity value (n+1) = (0+1) = 1. The spin state is singlet (lowest spin state).

The electronic configuration (EC) for low spin (LS) tetrahedral complexes with CFT and their corresponding spin multiplicity value and spin state can be calculated as follows:

For $3d^1$(LS), electronic representation – (e_g^1, t_{2g}^0), EC – (t_{2g}^0, e_g^1), number of unpaired electrons (n) = 1, spin multiplicity value (n+1) = (1+1) = 2. The spin state is doublet.

For $3d^2$(LS), electronic representation – ($e_g^{1.2}$, t_{2g}^0), EC – (t_{2g}^0, e_g^2), number of unpaired electron (n) = 2, spin multiplicity value (n+1) = (2+1) = 3. The spin state is triplet.

For $3d^3$(LS), electronic representation – ($e_g^{1.2,3}$, vt_{2g}^0), EC – (t_{2g}^0, e_g^3), number of unpaired electrons (n) = 1, spin multiplicity value (n+1) = (1+1) = 2. The spin state is doublet.

For $3d^4$(LS), electronic representation – ($e_g^{1,2,3,4}$, t_{2g}^0), EC – (t_{2g}^0, e_g^4), number of unpaired electrons (n) = 0, spin multiplicity value (n+1) = (0+1) = 1. The spin state is singlet (lowest spin state).

For $3d^5$(LS), electronic representation – ($e_g^{1,2,3,4}$, t_{2g}^5), EC – (t_{2g}^1, e_g^4), number of unpaired electrons (n) = 1, spin multiplicity value (n+1) = (1+1) = 2. The spin state is doublet.

For $3d^6$(LS), electronic representation – ($e_g^{1,2,3,4}$, $t_{2g}^{5,6}$), EC – (t_{2g}^2, e_g^4), number of unpaired electrons (n) = 2, spin multiplicity value (n+1) = (2+1) = 3. The spin state is triplet.

For $3d^7$(LS), electronic representation – ($e_g^{1.2,3,4}$, $t_{2g}^{5,6,7}$), EC – (t_{2g}^3, e_g^4), number of unpaired electrons (n) = 3, spin multiplicity value (n+1) = (3+1) = 4. The spin state is quartet.

For $3d^8$(LS), electronic representation – ($e_g^{1.2,3,4}$, $t_{2g}^{5,6,7,8}$), EC – (t_{2g}^4, e_g^4), number of unpaired electrons (n) = 2, spin multiplicity value (n+1) = (2+1) = 3. The spin state is triplet.

For $3d^9$(LS), electronic representation – ($e_g^{1,2,3,4}$, $t_{2g}^{5,6,7,8,9}$), EC – (t_{2g}^5, e_g^4), number of unpaired electrons (n) = 1, spin multiplicity value (n+1) = (1+1) = 2. The spin state is doublet.

For $3d^{10}$(LS), electronic representation – ($e_g^{1.2,3,4}$, $t_{2g}^{5,6,7,8,9,10}$), EC – (t_{2g}^6, e_g^4), number of unpaired electrons (n) = 0, spin multiplicity value (n+1) = (0+1) = 1. The pin state is singlet (lowest spin state).

From this data of, it is clear that both 3d^{5}(HS) octahedral and tetrahedral complexes can exhibit the highest spin state, which is known as a sextet because it corresponds to spin multiplicity value of 6 with 5 unpaired electrons 5. However, 3d^{6} (LS) octahedral, 3d^{10} (LS) octahedral, 3d^{10} (HS) octahedral, 3d^{10} (HS) tetrahedral, 3d^{4} (LS) tetrahedral, and 3d^{10} (LS) tetrahedral complexes can exhibit the lowest spin state, which is known as a singlet because it corresponds to a spin multiplicity value of 1 and 0 unpaired electrons.

QUESTIONS ON SPIN MULTIPLICITY

Q.1. The spectroscopic ground state term symbols for octahedral aqua complexes in Mn(II), Cr(III), and Cu(II), are (NET 2016)

a) ^{2}H, ^{4}F, and ^{2}D b) ^{6}S, ^{4}F, and ^{2}D c) ^{2}H, ^{2}H, and ^{2}D d) ^{6}S, ^{4}F, and ^{2}P

Ans: (b) ^{6}S, ^{4}F and ^{2}D [EC of Mn(II) is 3d^{5}, number of unpaired electrons (n) = 5, spin multiplicity = (n+1) = (5+1) =6; EC of Cr(III) is 3d^{3}, number of unpaired electrons (n) = 3, spin multiplicity = (n+1) = (3+1) =4 and EC of Cu(II) is 3d^{9}, number of unpaired electrons (n) = 1, spin multiplicity = (n+1) = (1+1) =2].

Q.2. The lowest energy term for the d^{6} configuration is (NET 2016)

a) ^{2}D b) ^{5}D c) ^{1}P d) ^{1}D

Ans: (b) ^{5}D [for EC d^{6}, number of unpaired electrons (n) = 4, spin multiplicity = (n+1) = (4+1) =5].

It can be expected that the time efficient innovative mnemonics described in this chapter will help students at undergraduate, senior undergraduate, and postgraduate level to predict spin multiplicity values and the corresponding spin state. This can be done using only the number of unpaired electrons (n) and without calculating the total spin quantum numbers (S). This has created an atomic symbol in inorganic chemistry's group theory. Experiments, *in vitro*, on 100 students, showed that by using these innovative formulae students could save up to 2–3 minutes in the examination hall when solving different problems on spin multiplicity and its related properties, such as the spin state and atomic symbol, in inorganic chemistry. On the basis of this, I can strongly recommend using these time efficient innovative mnemonics in inorganic chemistry.

CHAPTER 8

INNOVATIVE MNEMONICS FOR THE PREDICTION OF AROMATIC, ANTI AROMATIC AND NON-AROMATIC BEHAVIOUR OF SIMPLE ORGANIC COMPOUNDS

In this chapter, formulae based mnemonics have been highlighted by classifying the negative charge on a carbon atom (localized or delocalized) within the ring system in an innovative and time efficient manner. Here, I have tried to use 2 time efficient nmemonics by including 2 formulae to predict the aromatic and anti-aromatic behavior of simple organic compounds. This chapter includes innovative formulae that calculate the A value by just manipulating the number of π bonds within the ring system and the carbon's delocalized negative charge (DNC) with one (01). The cyclic or planar organic compound that is conjugated with an even number of A will be treated as aromatic and, when it has an odd number, it will be treated as an anti-aromatic. This chapter encourages students to solve multiple choice type questions (MCQs) on the aromaticity of organic compounds and its related properties at different competitive examinations in a time efficient manner.

The conventional methods to detect the planarity of organic compounds by predicting the hybridization state of carbon atoms in simple organic compounds and their relative aromaticity are time-consuming.[16] Keeping this in mind, in this innovative pedagogical chapter some innovative

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[16] Hückel, Erich, "Quantentheoretische Beiträge zum Benzolproblem I. Die Elektronenkonfiguration des Benzols undverwandter Verbindungen", *Z.Phys.* 70 (1931): 204 86; I. L. Finar, *Organic Chemistry 2* (Pearson: 2002), 606 637; R.T. Morrison, and R.N. Boyd, *Organic Chemistry* (1992), 1059 1061; T.W. Graham Solomons and C.B. Fryhle, *Organic Chemistry* (Wiley, India: 2012), 655-658; J.G. Smith, *Organic Chemistry* (2008), 616 619; Jerry March, *Advanced Organic Chemistry: Reaction, Mechanisms, and Structure.* (JOHN WILEY & SONS: 2005), 45; A. Bahl and B.S. Bahl, *A Text Book of Organic Chemistry* (S. Chand: 2016), 900 920.

mnemonics have been introduced, along with their omission behaviors, applications, and problems to make their discovery both time efficient and interesting.[17]

METHODOLOGY

1. Predicting the hybridization state of carbon atoms in different organic compounds

A. Classifying carbon's negative charge in organic compounds

The negative charge of a carbon atom from any organic compounds can be generally classified into two types: delocalized negative charge (DNC) and localized negative charge (LNC).

i) Delocalized negative charge (DNC): When the negative charge of a carbon atom from the ring system of an organic compound undergoes delocalization through conjugation then it should be treated as a delocalized negative charge (DNC). When a negative charge bearing carbon atom from the ring system of the organic compound is directly attached with single bonds at all ends, then it contains DNC and its negative charge is to be treated as a delocalized negative charge (DNC).

Example: In cyclopropenyl anions, cyclopentadienyl anions, and cycloheptatrienyl anions (Fig. 2.12, Fig. 2.13, and Fig. 2.14), the negative charge on C atom should be treated as a DNC because it is directly attached with single bonds from all sides of the ring system.

ii) Localized negative charge (LNC): When the negative charge from the carbon atom in the ring system of an organic compound does not undergo

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[17] A. Das *et. al*, "A rapid and innovative method for the identification of aromatic and anti-aromatic nature of organic compounds", *World Journal of Chemical Education* 1 (Sept 2013): 6-8, doi: 10.12691/wjce-1-1-2, http://pubs.sciepub.com/wjce/1/1/2/#; A. Das, "Innovative and Time Economic Pedagogical Views in Chemical Education: A Review Article", *World Journal of Chemical Education* 2 (July 2014): 29-38, doi:10.12691/wjce-2-3-1, http://pubs.sciepub.com/wjce/2/3/1/index.html#; A. Das, "Innovative Mnemonics in Chemical Education: Review Article", *African Journal of Chemical Education* 8 (July 2018): 144 189, https://www.ajol.info/index.php/ajce/article/view/176086; A. Das, "Innovative Mnemonics Make Chemical Education Time Economic: A Pedagogical Review Article", *World Journal of Chemical Education* 6 (Sept 2018): 154 174, doi:10.12691/wjce-6-4-2, http://pubs.sciepub.com/wjce/6/4/2/index.html.

delocalization through conjugation then it should be treated as a localized negative charge (LNC). When the negative charge bearing carbon atom is directly attached to the ring system with single and double bonds, it contains LNC and its negative charge should be treated as such.

B) Planarity in organic compounds

Planarity is vital when predicting the aromatic, anti-aromatic, and non-aromatic behavior of organic compounds. For aromatic and anti-aromatic behavior, the compound must be planar, whereas, non-planar organic compounds should be treated as nonaromatic in nature. The planarity of organic compounds depends on the nature of the hybridization state of their carbon atoms. When all the carbon atoms in an organic compound are in the same (sp^2) hybridization state then they are treated as planar but when they have both a sp^2 and a sp^3 hybridization state then they should be treated as non-planar. Predicting the hybridization state of organic compounds was discussed in Chapter 2 and the use of conventional formulae was discussed in Chapter 3.

2. Conventional methods to identify the aromatic and anti-aromatic behavior of organic compounds

Huckel first devised this in 1931.

i) To find the aromatic nature of an organic compound

a. cyclic b. planer, where all bonded atoms are in the same plane (sp^2 hybridized) c. aconjugated molecule with a conjugated π-electron system d. contains $(4n + 2)$ π electrons, where n is a positive integer (n=0, 1, 2, 3 etc.)

ii) To find the anti-aromatic nature of an organic compound

a. cyclic b. planer, where all bonded atoms are in the same plane (sp^2 hybridized) c. a conjugated molecule with a conjugated π-electron system d. contains $4n\pi$ electrons, where n is a positive integer (n = 0, 1, 2, 3 etc.).

iii) To find the non-aromatic nature of an organic compound

If a compound violates any one of these three conditions (a, b, or c) then it is non-aromatic in nature.

3. Innovative mnemonics to predict the aromatic and anti-aromatic behavior of simple organic compounds

These innovative mnemonics calculate the A value by manipulating the number of π bonds within the ring system and the delocalized negative charge of carbon atoms (DNC) to find the number of the electron pairs (e^-p) within the ring system. Organic compounds that are cyclic or planar (i.e., all the carbon atoms have the same state of hybridization, sp^2) conjugated with an even number of A value should be treated as aromatic in nature and those with an odd number should be treated as anti-aromatic.

i) Predicting aromatic behavior

The organic compound must be cyclic or planar (i.e. all the carbon atoms have the same state of hybridization) and conjugated with an even number for their A value, where $A = \pi b + e^-p$ (DNC) + 1 (constant); πb = number of π bonds within the ring system; and e^-p (DNC) = number of electron pairs within the ring system (delocalized negative charge on carbon atoms from the ring system). Here, each delocalized negative charge (DNC) should be treated as one electron pair (e^-p). If the value of A is an even number then it should be treated as an aromatic compound.

ii) Predicting anti-aromatic behavior

The organic compound must be cyclic or planar (i.e. all the carbon atoms have same state of hybridization) and conjugated with odd number for their A value, where $A = \pi b + e^-p$ (DNC) + 1 (constant); πb = number of π bonds within the ring system; and e^-p (DNC) = number of electron pairs within the ring system (delocalized negative charge on carbon atoms from the ring system). Here, each delocalized negative charge (DNC) should be treated as one electron pair (e^-p). If the A value of a certain organic compound comes out as an odd number then this compound should be treated as anti-aromatic.

iii) General conditions for the non-aromatic behavior of organic compounds:

Any compound that lacks one or more of the first three features (cyclic/conjugated/planar), and which may be acyclic/non-planar/non-conjugated, should be treated as nonaromatic.

Innovative formula: Evaluating the A value in order to predict the aromatic and anti-aromatic nature

$A = \pi b + e^{-}p\ (DNC) + 1\ (constant) = even\ no. = aromatic$

$A = \pi b + e^{-}p\ (DNC) + 1\ (constant) = odd\ no. = anti\text{-}aromatic$

Where πb = number of π bonds with in the ring system and e^{-} p (DNC) = number of electron pairs within the ring system (delocalized negative charge on carbon atoms of ring system). Here, each delocalized negative charge (DNC) should be treated as one electron pair (e^{-} p).

RESULTS AND DISCUSSION

1. Innovative mnemonics to predict the hybridization state (sp^2 and sp^3) of carbon atoms in organic compounds

Predicting the hybridization state (sp^2 and sp^3) of carbon atoms in organic compounds was discussed in Chapter 2.

2. Innovative mnemonics to predict the aromatic and anti-aromatic behavior of simple organic compounds

Innovative formula: Evaluating the A Value to predict the aromatic or anti-aromatic nature

$A = \pi b + e^{-}p\ (DNC) + 1\ (constant) = even\ no. = aromatic$

$A = \pi b + e^{-}p\ (DNC) + 1\ (constant) = odd\ no. = anti\text{-}aromatic$

Where πb = number of π bonds with in the ring system and e^{-} p (DNC) = number of electrons pairs within the ring system (delocalized negative charge of the carbon atoms in the ring system). Here, each delocalized negative charge (DNC) should be treated as one electrons pairs (e^{-}p). Any compound that lacks one or more of the first three features (i.e. it may be acyclic/non-planar/non-conjugated) should be treated as non-aromatic.

Example A: In cyclopropene, cyclopentadiene, and cycloheptatriene (Fig. 2.12, Fig. 2.13, and Fig. 2.14), the vertex carbon atom is in a sp^3 hybridization state (as discussed in Chapter 3). Here, in all cases, the presence of one sp^3 hybridized vertex carbon atom along with other sp^2 hybridized carbons makes cyclopropene, cyclopentadiene, and cycloheptatriene non-planar and, therefore, non-aromatic.

Example B: In cyclopropenyl anion, cyclopentadienyl anion, and cycloheptatrienyl anion (Fig. 2.12, Fig. 2.13, and Fig. 2.14), the vertex carbon atom bearing negative charge is in a sp^2 hybridization state (as discussed in Chapter 3). Here, in all cases, the vertex carbon atom's negative charge should be treated as a delocalized negative charge (DNC) and can be counted when predicting the A value and should not be counted when predicting the hybridization state. The presence of sp^2 hybridized carbons in cyclopropenyl anions, cyclopentadienyl anions, and cycloheptatrienyl anions makes them planar. Here, the A value for cyclopropenyl anion = πb + e^- p (DNC) + 1 (constant) = 1+1+1 = 3 (odd no.) = anti-aromatic; the A value for cyclopentadienyl anion = πb + e^- p (DNC) + 1 (constant) = 2+1+1 = 4 (even no.) = aromatic; and the A value for cycloheptatrienyl anion = πb + e^-p (DNC) + 1 (constant) = 3+1+1 = 5 (odd no.) = anti-aromatic.

Example C: In cyclopropenyl cation, cyclopentadienyl cation, and cycloheptatrienyl cation (Fig. 2.12, Fig. 2.13, and Fig. 2.14), the vertex carbon atom bearing positive charge is in a sp^2 hybridization state (as discussed in Chapter 3). The presence of sp^2 hybridized carbons in cyclopropenyl cations, cyclopentadienyl cations, and cycloheptatrienyl cations makes them planar. Here, the A value for cyclopropenyl cation = πb + e^-p (DNC) + 1 (constant) = 1+0+1 = 2 (even no.) = aromatic; the A value for cyclopentadienyl cation = πb + e^- p (DNC) + 1(constant) = 2+0+1 = 3 (odd no.) = anti-aromatic; and the A value for cycloheptatrienyl cation = πb + e^- p (DNC) + 1 (constant) = 3+0+1 = 4 (even no.) = aromatic.

In cyclobutadiene and cyclooctatetraene (Fig. 2.15), all carbon atoms are sp^2 hybridized (as discussed in Chapter 3), which makes them planar. Here, the A value for cyclobutadiene = πb + e^-p (DNC) + 1 (constant) = 2+0+1 = 3 (odd no.) = anti-aromatic and the A value for cyclooctatetraene = πb + e^-p (DNC) + 1 (constant) = 4+0+1 = 5 (odd no.) = anti-aromatic.

Examples of the aromatic, anti-aromatic and non-aromatic behavior of simple organic compounds are described in Table 8.6.

THE OMISSION BEHAVIOR OF AROMATIC AND NON-AROMATIC ORGANIC COMPOUNDS

There are some compounds that do not follow the above rules regarding their A value. Huckel is also not able to explain the aromatic or non-aromatic behavior of these compounds. These compounds have been represented below.

Cyclodecapentaene (Fig.8.25) is non-aromatic due to the interaction of hydrogen in 1 and 6. However, it is non-planar, although here $A = \pi b + e^{-}p$ (DNC) + 1 (constant) = 5 + 0 + 1 = 6 (even number).

Pyrene (Fig. 8.25) is a polycyclic aromatic hydrocarbon consisting of four fused benzene rings, which results in a flat aromatic system. It has 8 π bonds and zero (0) DNC. Here, A = 8 + 0 + 1 = 9 (odd number). However, it is aromatic instead of anti-aromatic because the double bonded C_{15}-C_{16} does not take part in its resonance.

APPLICATIONS FOR AROMATICITY IN ORGANIC CHEMISTRY

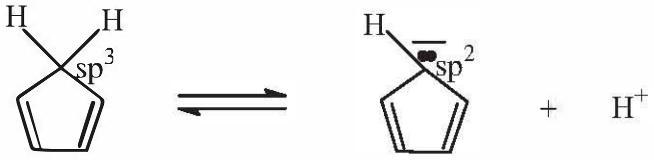
i) Predicting the stability and reactivity order of organic compounds with aromaticity.

The stability of organic compounds follows the order: aromatic > non-aromatic> anti-aromatic. Reactivity is inversely proportional to the stability so, therefore, reactivity follows the order, anti-aromatic > non-aromatic> aromatic.

Example A: cyclopropenyl cation (aromatic) > cyclopropene (non-aromatic) > cyclopropenyl anion (anti-aromatic) (Stability) and reactivity order is cyclopropenyl cation (aromatic) < cyclopropene (non-aromatic) < cyclopropenyl anion (anti-aromatic).

ii) Predicting the acidic character of organic compounds with aromaticity

Cyclopentadienyl anion (the conjugate base of cyclopentadiene) is aromatic, whereas cycloheptatrienyl anion (the conjugate base of cycloheptatriene) is anti-aromatic. The stability of organic compounds follows the order: aromatic > non-aromatic> anti-aromatic. Therefore, the conjugate base of cyclopentadiene is much more stable than the conjugate base of cycloheptatriene, as depicted below:

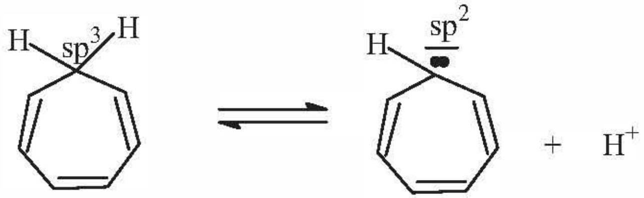


(Cyclopentadiene)
(Non Aromatic)

(Cyclopentadienyl anion)
(Aromatic)

(Conjugate Acid) (Conjugate Base)

A = 2 + 1 + 1(constant) = 4 (even no.) (aromatic)



(Cycloheptatriene)
(Non Aromatic)

(Cycloheptatrienyl anion)
(Anti Aromatic)

(Conjugate Acid) (Conjugate Base)

A = 3+ 1 + 1(constant) = 5 (odd no.) (anti-aromatic)

In the first case, due to the stability of the conjugate base (cyclopentadienyl anion) the equilibrium has shifted forward, which increases the concentration of H^+ (proton) as well as the acidity of cyclopentadiene. This is why cyclopentadiene is much more acidic than cycloheptatetraene.

iii) Predicting the stability and reactivity of organic compounds and aromaticity using molecular orbital theory (MOT)

- Stability $\propto$ number of filled bonding molecular orbitals (BMOs)
- For the same number of filled BMOs, stability $\propto$ 1 / number of electrons in anti-bonding molecular orbitals (ABMOs)

Example A: The decreasing order of stability among cyclopropenyl anion, cyclopropenyl radical, and cyclopropenyl cation:

cyclopropenyl cation > cyclopropenyl radical > cyclopropenyl anion. This is due to the different numbers of electrons in anti-bonding molecular orbitals (ABMOs) in cyclopropenyl anion, cyclopropenyl cation and cyclopropenyl radical where, in all cases, the number of filled bonding molecular orbital (FBMO) are the same (Fig. 8.26). Since reactivity is inversely proportional to stability, reactivity is in the following order: cyclopropenyl cation < cyclopropenyl radical < cyclopropenyl anion. This is because the increasing number of electrons in high-energy anti-bonding molecular orbitals (ABMOs) increases reactivity and thus decreases the stability of organic compounds.

Example B: The decreasing order of stability among cyclopentadienyl anion, cyclopentadienyl radical and cyclopentadienyl cation: cyclopentadienyl anion (FBMOs = 3) > cyclopentadienyl radical (FBMOs = 2) > cyclopentadienyl cation (FBMOs = 1).

Here, FBMOs = filled bonding molecular orbitals (Fig. 8.27).

QUESTIONS ON AROMATICITY

Q.1. Which one of the following chemical systems is non-aromatic?

a) Benzene b) Naphthalene c) Cyclopropenyl anion d) Cyclopentadiene

Ans: (d) Cyclopentadiene (the sp^3 hybridized C atom makes it non-planar and, therefore, non-aromatic)

Q.2. Which is the non-aromatic compound?

a) Cyclopentadiene b) Benzene c) Naphthalene d) None

Ans: (a) Cyclopentadiene (the sp^3 hybridized C atom makes it non-planar and, therefore, non-aromatic)

Q.3. Which one is more stable?

a) Cyclopentadienyl anion b) Cyclopentadiene c) Cyclopentadienyl cation d) None

Ans: (a) Cyclopentadienyl anion (Aromatic)

It can be expected that these 2 time efficient innovative mnemonics will help chemical education students at undergraduate, senior undergraduate, and postgraduate level to predict the aromatic and anti-aromatic behavior of organic compounds. Experiments, *in vitro,* on 100 students showed that these formulae could save students up to 4–5 minutes in the examination hall. On the basis of this, I can strongly recommend using these time efficient and innovative mnemonics.

CHAPTER 9

INNOVATIVE MNEMONICS FOR THE PREDICTION OF AROMATIC, ANTI AROMATIC AND NON-AROMATIC BEHAVIOUR OF HETEROCYCLIC COMPOUNDS

In this chapter, innovative and time efficient formulae-based nmemonics have used to classify a lone pair of electrons (localized or delocalized). I have tried to connect 2 time-efficient mnemonics by including 2 formulae to predict the aromatic and anti-aromatic behavior of heterocyclic compounds. This chapter includes innovative formulae that calculate the A value by just manipulating the number of π bonds within the ring system and the delocalized lone pair electron (DLP) with one (01). A heterocyclic compound that is cyclic and planar, when conjugated with an even number for its A value, will be treated as aromatic and, when it has an odd number for its A value, it will be treated as anti-aromatic. In a multi-heteroatom based heterocyclic compound, which contains both a delocalized lone pair electron (DLP) and a localized lone pair electron (LLP) based heteroatom, aromatic and anti-aromatic behavior will be predicted with respect to the DLP-based heteroatom only. When heterocyclic compounds contain both LLP-based heteroatoms then its aromaticity will be predicted using the heteroatom that contains the lowest position number as per its IUPAC nomenclature. Conventional methods for detecting the planarity of organic compounds using the hybridization state of carbon atoms in simple organic compounds and their relative aromaticity are time consuming.[18] Keeping this in mind, using my innovative pedagogy, innovative nmemonics have

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[18] Hückel, Erich, "Quantentheoretische Beiträge zum Benzolproblem I. Die Elektronenkonfiguration des Benzols undverwandter Verbindungen", *Z.Phys.* 70 (1931): 204 86; I. L. Finar, *Organic Chemistry 2* (Pearson: 2002), 606 637; R. T. Morrison, and R.N. Boyd, *Organic Chemistry* (1992), 1059-1061; T. W. Graham Solomons and C. B. Fryhle *Organic Chemistry* (Wiley, India: 2012), 655 658; J. G. Smith, *Organic Chemistry* (2008), 616 619; Jerry March, *Advanced Organic Chemistry: Reaction, Mechanisms, and Structure* (John Wiley and Sons: 2005), 45.

been introduced by classifying a lone pair of electrons as LLP and DLP, along with their omission behaviors, applications, and problems. This will mean that the detection of the aromaticity of heterocyclic compounds in different competitive examinations time efficient and interesting.[19]

METHODOLOGY

1. Predicting the heteroatom's hybridization state in different heterocyclic compounds.

A) Classifying a lone pair of electrons in heterocyclic compounds

A lone pair of electrons can be generally classified into two types: delocalized lone pair electrons (DLP) and localized lone pair electrons (LLP).

i) Delocalized lone pair electron (DLP): When the lone pair of electrons from a heteroatom undergo delocalization through conjugation then it should be treated as a delocalized lone pair electron (DLP).

A heteroatom (an atom containing a lone pair electro) that is directly attached with only single bonds at all ends is a DLP based heteroatom and its lone pair is to be treated as such.

Example: In Pyrrole (Fig. 2.16), the lone pair of N atoms should be treated as a DLP because it is directly attached to only three single bonds.

ii) Localized lone pair electron (LLP): When the lone pair of electrons of the heteroatom do not undergo delocalization through conjugation then it should be treated as a localized lone pair of electrons (LLP). A heteroatom (an atom containing a lone pair electron) that is directly attached with single and double bonds using the ring system is considered to be an LLP, which contains a heteroatom and its lone pair.

Example: In pyridine (Fig. 2.16), the lone pair of N atoms is to be treated as an LLP because it is directly attached with double and single bonds using the ring system.

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[19] A. Das, "Lone Pair Electron Discriminate Hybridization with Aromatic and Anti Aromatic behavior of Heterocyclic Compounds-Innovative Mnemonics", *World Journal of Chemical Education* 6 (April 2018): 95 101, doi: 10.12691/wjce-6-2 4, http://pubs.sciepub.com/wjce/6/2/4/.

B) Planarity of heterocyclic compounds

Planarity is one of the vital methods to predict the aromatic, anti-aromatic, and non-aromatic behavior of heterocyclic compounds or other organic compounds. For aromatic and anti-aromatic behaviors, the compound must be planar, whereas the non-planar compound is non-aromatic in nature. The planarity of heterocyclic compounds depends on the nature of the hybridization state of carbon and the heteroatoms present. When all atoms (carbon and hetero) in the heterocyclic compound are sp^2 hybridized then they are planar but when there is a mixture of sp^2 and sp^3 hybridization states then it is treated as non-planar.

C) The conventional method for predicting the hybridization state of a heteroatom in heterocyclic compounds.

The hybridization state of a molecule can be calculated by the formula: $P = 1/2\ (V+MA-C+A)$, where V = number of valance electrons in the central atom; MA = number of surrounding monovalent atoms;

C = cationic charge; A = anionic charge; P = power of the hybridization state of the central atom.

D) An innovative mnemonic to predict the hybridization state of a heteroatom in order to forecast the planarity of different heterocyclic compounds.

Prediction of sp^2 and sp^3 hybridization states:

Power of the hybridization state of the heteroatom (P_{Hyb}) = (T_{SLLP}) − 1, where P_{Hyb} = power of the hybridization state of the heteroatom; T_{SLLP} = (total no of σ bonds around each central atom + localized lone pair electron); S = number of σ bonds around each central atom; LLP = localized lone pair of electrons.

If the power of the hybridization state (P_{Hyb}) is ●3, ●2, and ●1 then the hybridization state will be sp^3, sp^2, and sp, respectively. All single (-) bonds are σ bonds and, in the double bond (=), there is one σ and one π. In addition to these, each localized lone pair electron (LLP) can be treated as one σ bond.[7]

2. Huckel first devised the identification of the aromatic and anti-aromatic behavior of organic compounds in 1931.

A) Conventional methods:

i) Aromatic nature of an organic compound

1. Cyclic molecule

2. Planer molecule in which all bonded atoms lie on the same plane (sp^2 hybridized)

3. Conjugated molecule with conjugated π-electron system

4. Contains $(4n + 2)$ π electrons, where n is a positive integer (n = 0, 1, 2, 3 etc.)

ii) Anti-aromatic nature of an organic compound:

1. Cyclic molecule
2. Planer molecule in which all bonded atoms lie in the same plane (sp^2 hybridized)
3. A conjugated molecule with a conjugated π-electron system
4. $4n\pi$ electrons, where n is a positive integer (n = 0, 1, 2, 3 etc.)

iii) Non-aromatic nature of an organic compound:

If a compound violates any one of these three conditions (1, 2, or 3) then it is non-aromatic in nature.

B) An innovative nmemonic for the aromatic and anti-aromatic behavior of heterocyclic compounds:

The innovative mnemonic calculates the A value by just manipulating the number of π bonds within the ring system and the delocalized lone pair electron (DLP) with one (●1).

The heterocyclic compound, whether it is cyclic, planar, or conjugated (i.e., all the carbon atoms have the same state of hybridization, sp^2): an even number for its "A" value, which will be treated as aromatic in nature and, an odd number for its A value will be treated as an anti-aromatic in nature.

i) Predicting aromatic behavior:

In the first case, the compound must be cyclic or planar (i.e., all the carbon atoms have the same state of hybridization) and conjugated with an even number of A value, where [A = πb+DLP+1(constant)]. πb = number of π bonds within the ring system and DLP = delocalized lone pair of electrons (lone pair of electrons in the heteroatom, which undergo the delocalization).

If the value of A is an even number then this compound will be treated as aromatic.

ii) Predicting anti-aromatic behavior:

In the second case, the compound must be cyclic or planar (i.e., all the carbon atoms have the same state of hybridization) and conjugated with an odd number in its A value, where [A = πb+DLP+1(constant)]. Where, πb = number of π bonds within the ring system and DLP = delocalized lone pair of electrons.

If the value of A is an odd number then this compound will be treated as anti-aromatic.

iii) General conditions for the non-aromatic behavior of organic compounds:

Any compound that lacks one or more of the above features (e.g., acyclic/non-planar/non-conjugated) means it will be treated as nonaromatic. In this case, the A value may be an even or an odd number. It should be noted that in the case of some heterocyclic compounds, which contain both DLP and LLP heteroatoms, aromatic and anti-aromatic behavior should be predicted with respect to the DLP-based heteroatom only. In the case of a multi-heteroatom based heterocyclic compound, which contain both DLP and LLP heteroatoms, aromatic and anti-aromatic behavior should be predicted with respect to the DLP-based heteroatom only. However, when heterocyclic compounds contain LLP-based heteroatoms, then the aromaticity should be predicted with respect to the heteroatom that has the lowest position according to the IUPAC nomenclature.

RESULTS AND DISCUSSION

1. Predicting the hybridization state (sp^2 and sp^3) of a heteroatom in heterocyclic compounds.

The hybridization state of a heteroatom in a heterocyclic compound can be calculated from the total number of σ bonds around the heteroatom and the number of localized lone pairs of electrons (T_{SLLP}) on the heteroatom. Subtract one from the total value of T_{SLLP} to get the hybridization state (sp^2 and sp^3) of the heteroatom in the heterocyclic compound.

Examples that predict the hybridization state of a heteroatom in heterocyclic compounds containing one, two, or more of the same or a different number of heteroatoms from the corresponding T_{SLLP} value (total number of σ bonds around the central atom + localized lone pair of electrons on the central atom) of the central atom have been explored in Table 2.3.

2. An innovative mnemonic for the aromatic and anti-aromatic behavior of heterocyclic compounds.

The following is an innovative mnemonic to calculate the "A" value by just manipulating the number of π bonds within the ring system and the delocalized lone pair electron (DLP) with one.

If the heterocyclic compound, whether it is cyclic, planar, or conjugated (i.e., all the carbon atoms have the same state of hybridization, sp^2), has an even number for its "A" value, it will be treated as aromatic in nature and, if it has an odd number, then it will be treated as an anti-aromatic in nature. The aromatic, anti-aromatic, and non-aromatic behaviors of some heterocyclic compounds have been illustrated below and in Table 9.7.

Example A: Pyridine is a cyclic, planar, and conjugated heterocyclic compound. In pyridine (Fig. 2.16), the lone pair of "N" atoms is to be treated as a localized lone pair of electrons (LLP) because it is directly attached with double and single bonds using the ring system. Therefore, it is used to calculate power of the hybridization state, $(P_{Hyb}) = (T_{SLLP}) - 1$, and to predict the hybridization state of the heteroatom "N" in pyridine. This LLP is not to be used to predict the "A" value [$A = \pi b + DLP + 1$(constant) to find the aromaticity of the heterocyclic compound. In pyridine, there are two σ bonds and one LLP (localized lone pair electrons) around "N". Hence, the power of the hybridization state of "N" in pyridine is $(P_{Hyb}) = (T_{SLLP}) - 1 = (2+1)-1 = 2$ (sp^2-N). All five carbon atoms are in the same hybridization state (sp^2); this means that pyridine is planar. Here, A = πb+DLP+1(constant) = 3 + 0 + 1 (constant) = 4 (even no.). Therefore, pyridine is aromatic in nature. πb = number of π bonds within the ring system and DLP = delocalized lone pair electron (a lone pair of electrons from the heteroatom that are directly attached with single bonds within the ring system).

Example B: Pyrrole is a cyclic, planar, and conjugated heterocyclic compound. In pyrrole (Fig. 2.16), the lone pair of N atoms is to be treated as a DLP because it is directly attached with only three single bonds. It can be used to calculate the "A" value [A = πb+DLP+1(constant)] of the aromaticity of a heterocyclic compound. However, it cannot be used to calculate the power of the hybridization state, (P_{Hyb}) = (T_{SLLP}) – 1, or to predict the hybridization state of the heteroatom "N" in pyrrole. Here, around the "N", there are three σ bonds and zero LLP (localized lone pair electrons). Therefore, the power of the hybridization state of "N is in pyrrole, (P_{Hyb}) = (T_{SLLP}) – 1 = (3+0)-1 = 2 (sp^2-N). All four carbon atoms are in the same hybridization state of sp^2; this means that pyrrole is planar. A = πb+DLP+1(constant) = 2 + 1 + 1 (constant) = 4 (even no.); therefore, pyrrole is aromatic in nature. πb = number of π bond within the ring system and DLP = Delocalized lone pair electron (the lone pair electrons of a heteroatom which are directly attached with single bonds within the ring system).

Example C: Quinoline is a cyclic, planar, and conjugated heterocyclic compound. In quinoline (Fig. 2.16), the lone pair of N atoms is to be treated as a localized lone pair of electrons (LLP) because, it is directly attached with double and single bonds using the ring system; therefore, it can be used to calculate the power of the hybridization state, (P_{Hyb}) = (T_{SLLP}) – 1, and to predict the hybridization state of the heteroatom N in quinoline. This LLP should not be used to predict the A value [A = πb+DLP+1(constant)] in the aromaticity of a heterocyclic compound. In quinoline, there are two σ bonds and one LLP (localized lone pair of electrons) around the "N". Therefore, the power of the hybridization state of "N" in quinolone is (P_{Hyb}) = (T_{SLLP}) – 1 = (2+1)-1 = 2 (sp^2-N). All of the carbon atoms are in the same hybridization state of sp^2; this means that quinoline is planar. A = πb+DLP+1(constant) = 5 + 0 + 1 (constant) = 6 (even no.); hence, quinoline is aromatic in nature. πb = number of π bonds within the ring system and DLP = delocalized lone pair of electrons (the lone pair of electrons in the heteroatom which are directly attached with single bonds within the ring system).

Example D: Aziridine (Fig. 2.17) is a cyclic, non-planar, non-conjugated heterocyclic compound. The N atom is surrounded by three σ bonds and one LLP (localized lone pair electrons). Therefore, the power of the hybridization state of "N" in aziridine is (P_{Hyb}) = (T_{SLLP}) – 1 = (3+1)-1 = 3 (sp^3-N). This means that it is non-planar and non-aromatic.

Example E: Oxetane (Fig. 2.17) is a cyclic, non-planar, non-conjugated heterocyclic compound. The O atom is surrounded by two σ bonds and two LLPs (localized lone pair of electrons). Therefore, the power of the hybridization state of "O" in oxetane is (P_{Hyb}) = (T_{SLLP}) – 1 = (2+2)-1 = 3 (sp^3-O). This means that it is non-planar and non-aromatic.

OMISSION BEHAVIOR OF HETEROCYCLIC COMPOUNDS WITH RESPECT TO AROMATIC, ANTI-AROMATIC AND NON-AROMATIC BEHAVIOUR

i) A heterocyclic compound, containing both DLP and LLP heteroatoms:

In a multi-heteroatom heterocyclic compound, the aromatic and anti-aromatic behavior should only be predicted in the DLP-based heteroatom.

Example A: Benzothiazole (Fig. 9.28) is a multi-heteroatom heterocyclic compound. For N, DLP = 0, LLP = 1 and, for S, DLP = 1, LLP =1. In this case, the A value should be calculated only in S and not in N. Here, A = 4 + 1 + 1 = 6 (even no.) = aromatic.

When heterocyclic compounds contain LLP-based heteroatoms then the aromaticity should be predicted using the heteroatom that has the lowest number in the IUPAC nomenclature.

Example B: Imidazole (Fig. 9.28) is a multi-heteroatom heterocyclic compound, where N1 is a DLP-based heteroatom and N3 is LLP-based heteroatom. In this case, the aromaticity should be predicted based on the DLP-based heteroatom, N1. For N1, A = πb+DLP+1(constant) = 2+1+1 = 4 (even no.) = aromatic.

Example C: Pyrimidine (Fig. 9.28) is a multi-heteroatom heterocyclic compound, where both N1 and N3 are in the same environment (LLP-based heteroatoms). In this case, the aromaticity should be predicted using N1 (lowest possible position number as per IUPAC nomenclature). For N1, A = πb+DLP+1(constant) = 3+0+1 = 4 (even no.) = aromatic.

ii) Heterocyclic compounds containing different DLP-based heteroatoms (one also contains vacant d orbitals):

Example D: Phenothiazine (Fig. 9.29) contains two DLP-based heteroatoms, N and S. Due to the fact that S has vacant d orbitals, the A value should be predicted using the DLP-based S heteroatom. This is because it only contains vacant d orbitals. Here, A = πb + DLP + 1(constant) = 6 +1+1 = 8 (even no.) = aromatic.

iii) Heterocyclic compounds containing DLP-based heteroatoms with no d orbitals:

The omission behavior of some heterocyclic compounds, such as 1,2-dioxin, 1,4-dioxin, and dibenzo-1.4-dioxin (Fig. 9.29), can be observed when there are at least 2 heteroatoms (alike or different) that do not have any d orbitals (such as O.) and they are in a DLP-based environment in the ring system. These molecules have been studied with advanced molecular orbital techniques known as “ab initio calculations”. “Ab initio quantum chemistry methods” are computational approaches that are based on quantum chemistry.[20]

In 1,2-dioxins, 1,4-dioxins, and dibenzo-1.4-dioxins (Fig. 9.29), DLP-based O atoms will be found in all the molecules but they will still be non-aromatic due to the fact that free electron delocalization is restricted. This makes them non-conjugated. The π electrons from the carbon bonds and the lone pair of electrons on the oxygen atoms do not overlap to a significant degree due to the absence of vacant d orbitals in both O atoms (pπ-dπ overlap is not possible in conjugation). This makes these molecules non-conjugated and thus allows them to become non-aromatic instead of aromatic (A value = even no.).

In heterocyclic compounds where there are 2 DLP-based N atoms instead of 2 DLP-based O atoms or there is a DLP N atom and a DLP O atom, the same phenomena of non-aromatic behavior will be observed. This is because both N and O atoms do not have any vacant d orbitals and, therefore, the pπ-dπ overlap is not possible in conjugation.

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[20] Levine, Ira N. “Quantum Chemistry”. *Englewood Cliffs, New Jersey: Prentice Hall*. (1991): 455 544

iv) Heterocyclic compounds containing DLP-based heteroatoms with vacant d orbitals:

1,4-dithiin and 1,2-dithiin heterocyclic compounds (Fig. 9.29) are anti-aromatic. Both S atoms, because they have vacant d orbitals, contain a DLP and an LLP, and the DLPs of both S atoms participate in the delocalization. To predict the A value both DLP (DLP = 2) must be considered. Here, $A = \pi b + DLP + 1$ (Constant) = 2 + 2 + 1 = 5 (odd no.) = Anti-aromatic

APPLICATIONS OF AROMATICITY IN HETEROCYCLIC ORGANIC CHEMISTRY

i) To predict the basic character of a heterocyclic compound:

A delocalized lone pair of electrons (DLP) on the nitrogen atom from a heterocyclic compound with aromaticity decreases the basic nature of the heterocyclic compound, while a localized lone pair of electrons (LLP) increases its basic character.

Example A: Pyridine (LLP = 01, DLP = 0) is more basic than pyrrole (DLP = 01, LLP = 0). This is because the lone pair of N in pyrrole is delocalized (DLP) through resonance. This means that they cannot be donated for protonation, while the lone pair of N in pyridine is localized (LLP) and ready for donation.

Example B: Pyridine (LLP = 01, DLP = 0) is more basic than indole (DLP = 01, LLP = 0). This is because the lone pair of N in indole is in delocalized (DLP) through resonance. This means that they cannot be donated or protonated, while the lone pair of N in pyridine is localized (LLP) and ready for donation.

Example C: Furan (LLP = 01, DLP = 01) is more basic that pyrrole (DLP = 1, LLP = 0). This is due to the presence of an electronegative oxygen atom (E.N. = 3.5), which is higher than nitrogen (E.N. = 3.0). This decreases the delocalization tendency of the lone pair of electrons with regard to resonance. Therefore, the electron density on the heteroatom oxygen in furan is increased.

ii) To predict the stability and reactivity of different heterocyclic compounds using aromaticity:

When the nature of the heterocyclic (aromatic, anti-aromatic or non-aromatic nature) has been predicted, then the issue of stability and reactivity can be easily solved. The order of stability is aromatic > non-aromatic> anti-aromatic. The order of reactivity is anti-aromatic > non-aromatic> aromatic because the stability is inversely proportional to its reactivity.

QUESTIONS ON AROMATICITY

Q.1. Which one of the following chemical system is nonaromatic? (Karnataka NEET 2013)

a) benzene b) naphthalene c) thiophene d) cyclopentadiene

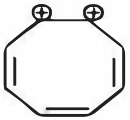
Ans: (d) cyclopentadiene (the sp^3 hybridized C atom makes it non-planar and, therefore, non-aromatic)

Q.2. Which is the nonaromatic compound? (AIEEE 2011)

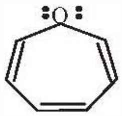
a) cyclopentadiene b) thiophene c) naphthalene d) none

Ans: (a) cyclopentadiene (the sp^3 hybridized C atom makes it non-planar and, therefore, non-aromatic)

Q.3. The correct statement about following species is (NET 2018)



A

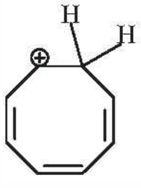


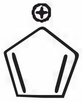
B

a) Both A and B are aromatic; b) A is aromatic and B is anti-aromatic; c) A non-aromatic and B is anti-aromatic d) A is aromatic and B is homo-aromatic

Ans: (b) A is aromatic and B is anti-aromatic [for species A, DNC = 0, “A” value = 3+0+1 = 4 (even number = aromatic) and for species B, LLP =1, DLP = 1, A value = 3+1+1 = 5 (odd number = anti-aromatic)]

Q.4. Among the carbocations given below (NET 2011)


A


B


C

a) A is homoaromatic, B is anti-aromatic, and C is aromatic; b) A is aromatic, B is anti-aromatic, and C is homoaromatic; c) A is anti-aromatic, B is aromatic and C is homoaromatic; d) A is homoaromatic, B is aromatic and C is anti-aromatic.

Ans: (a) A is homoaromatic, B is anti-aromatic, and C is aromatic [sp^3 hybridized carbon atom in A makes it homoaromatic; for B, "A" value = 2+0+1 = 3 (odd number – anti-aromatic); and for species C, "A" value = 1+0+1 = 2 (even number - aromatic)].

Q.5. Which one of the following pairs is more basic?

i) pyridine and pyrrole ii) pyridine and indole iii) furan and pyrrole

Ans: i) pyridine > pyrrole ii) pyridine > indole iii) furan > pyrrole

It can be expected that these time efficient innovative mnemonics will help students of chemical education from undergraduate to postgraduate level to predict the hybridization state of the heteroatom, and identify the aromatic and anti-aromatic behavior of heterocyclic compounds by classifying the lone pair of electrons present. Experiments, *in vitro*, on 100 students showed that, by using these formulae, they could save up to 5–10 minutes in the examination hall.

CHAPTER 10

INNOVATIVE MNEMONICS FOR THE CALCULATION OF CHEMICAL BONDS IN ALKENES

Chapter 10 is totally different from the others. In this chapter, some quickly innovative formulae have been proposed to calculate the number of chemical bonds (π-bonds, σ-bonds, single and double bonds) in aliphatic unsaturated open chain and cyclic olefinic hydrocarbons without drawing their exact structures. This chapter helps students to solve multiple choice type questions (MCQs) and calculate the chemical bonds in alkenes during different competitive examinations in a time efficient manner.

The molecular formula, which is used to define a very large number of hydrocarbon units (H & C) in alkenes, is a Herculean task for students and educators, as it requires them to calculate the number of chemical bonds by drawing their precise structures. Badertscher *et.al.* studied a novel formula to characterize the degree of unsaturation in organic molecules.[21] However, no work has yet been undertaken to calculate the number of chemical bonds in the open chain olefinic system with complex molecular formulae (e.g. $C_{176}H_{250}$ and $C_{2000}H_{2000}$). This makes the author's study extremely timely and necessary. Some rapid innovative mnemonics have been introduced to calculate the number of chemical bonds (e.g. π-bonds, σ-bonds, single and double bonds) by simply counting the number of carbon and hydrogen atoms using six innovative formulae for aliphatic unsaturated open chain and cyclic olefinic hydrocarbons.[22, 23]

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[21] M. Badertscher *et .al.*, "A Novel Formalism To Characterize the Degree of Unsaturation of Organic Molecules", *J. Chem. Inf. Comput. Sci.* 41 (May 2001): 889 893, doi: 10.1021/ci000135o,
https://pubs.acs.org/doi/abs/10.1021%2Fci000135o.

[22] A. Das *et. al.*, "Rapid calculation of the number of π-bonds, σ-bonds, single and double bonds in the aliphatic unsaturated open-chain and cyclic olefinic

METHODOLOGY

A. Innovative mnemonics to calculate the chemical bonds in open chain olefinic hydrocarbons.

(i) Calculating π-bonds and double bonds (P):

The number of π bonds or double bonds in an olefin is $P = [(2X-Y)/2] + 1$, where X = number of carbon atoms, Y = number of hydrogen atoms, and P = number of π bonds/double bonds.

(ii) Calculating σ-bonds (S):

The number of σ bonds for a straight chain olefin is $S = [X + Y - 1]$, where X = number of carbon atoms, Y = number of hydrogen atoms, and S = number of sigma bonds (σ-bonds).

(iii) Calculating single bonds (A):

The total number of single bond for a straight chain olefin is $A = [(3Y/2)-2]$, where A = number of single bonds and Y is the number of hydrogen atoms.

B. Innovative mnemonics to calculate the chemical bonds in cyclic aliphatic olefinic hydrocarbons.

(i) Calculation of π-bonds and double bonds (P_c):

The number of π bonds or double bonds in an aliphatic cyclic olefin is **$P_c = [(2X-Y)/2]$,** where X = number of carbon atoms, Y = number of hydrogen atoms, and P_c = number of π bonds or double bonds in the cyclic olefinic system.

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hydrocarbons", *Education in Chemical Science and Technology* 2 (Aug 2014):41 46.

[23] A. Das, "A Review of Time Economic Innovative Mnemonics In Chemical Education", *International Journal of Physics & Chemistry Education* 10 (June 2018): 27 40, doi: 10.12973/ijpce/81589, http://www.ijpce.org/A-Review-of-Time-Economic-Innovative-Mnemonics-in-Chemical-Education,81589,0,2.html.

(ii) Calculating σ-bonds (S_c):

The number of σ bonds in an aliphatic cyclic olefin is $S_c = [X + Y]$; where X = number of carbon atoms, Y = number of hydrogen atoms, and S_c = number of sigma bonds (σ-bonds) in the cyclic olefinic system.

(iii) Calculating single bonds (A_c):

The total number of single bonds in aliphatic cyclic olefin can be calculated using the formula

$A_c = [3Y/2]$, where A_c = number of single bonds and y is the number of hydrogen atoms in aliphatic cyclic olefin.

RESULTS AND DISCUSSION

Chemical bonds (π-bonds, σ-bonds, single and double bonds) in open chain and cyclic olefinic hydrocarbons that have complex molecular formulae (e.g. $C_{176}H_{250}$ and $C_{2000}H_{2000}$) can be calculated without drawing their structures by using different methods that only focus on the number of carbon and hydrogen atoms.

A. Innovative mnemonics to calculate chemical bonds in open chain olefinic hydrocarbons.

Example A: For C_2H_4 ($H_2C{=}CH_2$), number of carbon atoms, X = 2 and number of hydrogen atoms, Y = 4, the, number of π bonds will be $P = [(2X\text{-}Y)/2+1] = 1$; σ bonds, $S = [X+Y\text{-}1] = 5$; single bonds, $A = [(3Y/2)\text{-}2] = 4$; and double bonds, $= [(2X\text{-}Y)/2 + 1] = 1$.

Example B: For C_3H_6 ($H_2C{=}CH\text{-}CH_3$), number of carbon atoms, X = 3 and number of hydrogen atoms, Y = 6, the number of π bond will be $P = [(2X\text{-}Y)/2+1] = 1$; σ bonds, $S = [X+Y\text{-}1] = 8$; single bonds, $A = [(3Y/2)\text{-}2] = 7$; and double bonds $= [(2X\text{-}Y)/2 + 1] = 1$.

Adequate examples to calculate the chemical bonds (π bonds, σ bonds, single and double bonds) in open chain olefinic hydrocarbons without drawing their structures have been illustrated in Table 10.8.

B. Innovative mnemonics to calculate chemical bonds in cyclic olefinic hydrocarbons.

Example C: For cyclopropene (C_3H_4), number of carbon atoms, X = 3 and number of hydrogen atoms, Y = 4, the number of π bonds will be (P_c) = [(2X-Y)/2] = 1; σ bonds, (S_c) = [X+Y] = 7; single bonds, (A_c) = [(3Y/2)] = 6; and double bonds = [(2X-Y)/2] = 1.

Adequate examples to calculate chemical bonds (π bonds, σ bonds, single and double bonds) in cyclic olefinic hydrocarbons without drawing their structures have been illustrated in Table 10.9.

It can be expected that these time efficient innovative mnemonics will go a long way to help chemistry students from undergraduate to postgraduate level. Experiments *in vitro* on 100 students, showed that by using these formulae students could save up to 3–5 minutes in the examination hall. On the basis of this, I can strongly recommend using these methods in organic chemical education.

CHAPTER 11

INNOVATIVE MNEMONICS FOR THE CALCULATION OF CHEMICAL BONDS IN ALKYNES

The previous chapter proposed some speedy innovative formulae to calculate the number of chemical bonds (π-bonds, σ-bonds, single and double bonds) in aliphatic unsaturated open chain and cyclic olefinic hydrocarbons without drawing their exact structures. Now, Chapter 11 will present some quick innovative formulae to calculate the number of chemical bonds (π-bonds, σ-bonds, single and triple bonds) in aliphatic unsaturated open chain alkynes and cycloalkynes without drawing their structures. It will also help students to solve multiple-choice questions (MCQs) in different competitive examinations that require the chemical bonds in alkynes to be calculated in a time efficient manner without drawing their correct structures. The molecular formula that defines a large number of hydrocarbon units (H & C) in alkynes presents a formidable task for students and educators because, in order to calculate the number of chemical bonds, it requires their precise structures to be drawn. Keeping this in mind, some hasty innovative nmemonics have been introduced to calculate the number of chemical bonds (such as π-bonds, σ-bonds, single and triple bonds) by merely counting number of carbon and hydrogen atoms in aliphatic unsaturated open chain and cycloalkynes using 8 innovative formulae.[24, 25, 26]

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[24] A. Das *et al.*, "Rapid calculation of the number of π-bonds, σ-bonds, single and triple bonds in aliphatic Unsaturated open chain and cycloalkynes", *World Journal of Chemical Education* 2 (Dec 2013): 1 3, doi:10.12691/wjce-2-1-1, http://pubs.sciepub.com/wjce/2/1/1/#.

[25] A. Das, "A Review of Time Economic Innovative Mnemonics in Chemical Education", *International Journal of Physics & Chemistry Education* 10 (June 2018): 27 40, doi: 10.12973/ijpce/81589, http://www.ijpce.org/A-Review-of-Time-Economic-Innovative-Mnemonics-in-Chemical-Education,81589,0,2.html.

METHODOLOGY

A. Innovative mnemonics to calculate chemical bonds in open chain aliphatic alkynes

(i) π-bonds (P):

The number of π bonds in an aliphatic open chain alkyne is $P= [(2X-Y)/2] + 1$, where X = number of carbon atoms, Y = number of hydrogen atoms, and P = number of π bonds.

(ii) σ-bonds (S):

The number of σ bonds in an aliphatic open chain alkyne is $S = [X + Y - 1]$, where X = number of carbon atoms, Y = number of hydrogen atoms, and S = number of sigma bonds (σ-bonds).

(iii) Single bonds (A):

The total number of single bond for an aliphatic open chain alkyne, where there are one or more than one triple bonds is $A = [\{(2X+5Y)/2\} - 3]/2$, where A = number of single bonds, X = number of carbon atoms, and Y = number of hydrogen atoms.

(iv) Triple bonds (T):

In the first case, we have to count the number of carbon atoms (X) and the number of hydrogen atoms (Y) in a given unsaturated hydrocarbon with triple bonds. The formula to calculate the number of triple bonds in an aliphatic open chain alkyne, where there are one or more than one triple bond is $T = [\{(2X-Y)/2\} + 1]/2$, where X = number of carbon atoms, Y = number of hydrogen atoms, and T = number of triple bonds.

B. Innovative mnemonics to calculate the chemical bonds in cycloalkynes

(i) π-bonds (P_c):

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[26] A. Das, "Innovative Mnemonics Make Chemical Education Time Economic: A Pedagogical Review Article", *World Journal of Chemical Education* 6 (Sept 2018): 154 174, doi:10.12691/wjce-6-4-2, http://pubs.sciepub.com/wjce/6/4/2/index.html

First, count the number of carbon atoms (X) and hydrogen atoms (Y) in the given unsaturated cycloalkyne. The formula to calculate the number of π bonds in an aliphatic cycloalkyne is $P_c = [(2X-Y)/2]$, where X = number of carbon atoms, Y = number of hydrogen atoms, and P_c = number of π bonds in the cycloalkyne system.

(ii) σ-bonds (S_c):

The number of σ bonds in an aliphatic cycloalkyne is $S_c = [X + Y]$, where X = number of carbon atoms, Y = number of hydrogen atoms, and S_c = number of sigma bonds (σ-bonds) in the cycloalkyne system.

(iii) Single bonds (A_c):

The total number of single bond in an aliphatic cycloalkyne is $A_c = [\{(2X+5Y)/2\}]/2$, where A_c = number of single bonds in cycloalkyne, X = number of carbon atoms, and Y = number of hydrogen atoms.

(iv) Triple bonds (T):

The number of triple bonds is $T_c = [\{(2X-Y)/2\}]/2$, where X = number of carbon atoms, Y = number of hydrogen atoms, and T_c = number of the triple bond.

RESULTS AND DISCUSSION

Chemical bonds (π-bonds, σ-bonds, single and triple bonds) in open chain cycloalkynes that have a complex molecular formula (such as $C_{15}H_{28}$ or $C_{16}H_{30}$) can be calculated without drawing their literal structures by using different formulae that only focus on the number of carbon and hydrogen atoms.

C. Innovative mnemonics to calculate the chemical bonds in open chain aliphatic alkynes

Example A: For $C_{10}H_{18}$, find the number of carbon atoms X = 10, and the number of hydrogen atoms Y = 18; then for the number of π bonds use $P = [(2X-Y)/2+1] = 2$; σ bonds, $S = [X+Y-1] = 27$; single bonds, $A = [\{(2X+5Y)/2\}-3]/2 = 26$; and triple bonds, $T = [(2X-Y)/2 + 1] / 2 = 1$.

Example B: For $C_{11}H_{20}$, find the number of carbon atoms X = 11, and the number of hydrogen atoms Y = 20; then for the number of π bonds use $P = [(2X-Y)/2+1] = 2$; σ bonds, $S = [X+Y-1] = 30$; single bonds, $A = [\{(2X+5Y)/2\}-3]/2 = 29$; and triple bonds, $T = [(2X-Y)/2 + 1] / 2 = 1$.

Examples of calculations for chemical bonds (π bonds, σ bonds, single and triple bonds) in open chain alkynes without drawing their exact structures have been illustrated in Table 11.10.

D. Innovative mnemonics to calculate chemical bonds in cycloalkynes

Example C: For cycloheptyne (C_7H_{10}) use X =7, Y = 10, and then to find the number of π bonds use (P_c) = [(2X-Y)/2] = (2x7-10) / 2 = 2; σ bonds (S_c) = [X + Y] = (7+10) = 17; single bonds (A_c) = [{(2X+5Y)/2}]/2 = [{(2x7+5x10)/2}]/2 = 32/2 = 16; and triple bonds (T_c) = [{(2X-Y)/2}]/2 = [{(2 x 7 – 10)/2}] / 2 = 2/2 = 1.

THE APPLICATION OF MNEMONICS WHEN USING ALKENES AND ALKYNES TO DESIGN CBL ACTIVITY

As described in Chapters 10 and 11, the use of mnemonics are helpful when calculating the bonds in both alkene and the alkyne system, designing computer-based learning (CBL) activities, and developing computer programs to produce chemistry educational software tools for chemistry, such as "Hydrocarbons Parser".[27] This tool validates hydrocarbon formulae by storing these in an array and mapping their elements to a PHP regular expression pattern. This tool is used to count chemical bonds, degrees of unsaturation (DoU), discriminate between functional isomers, and predict physical properties. All this is done without consulting molecular orbital theory or a chemical database.

This tool will encourage educators, scholars, and chemistry students to calculate the chemical bonds in the alkene and alkyne system. Data miners, computational chemists, chemical engineers, and chemists can also use this tool.

It can be expected that these time efficient innovative mnemonics to calculate the chemical bonds in open-chain cycloalkynes without drawing their precise structures will go a long way to help chemistry students from undergraduate to postgraduate level. Experiments *in vitro* on 100 students showed that, by using these formulae, 3 to 5 minutes could be saved in the examination hall. On the basis of this, I can strongly recommend using mnemonics in organic chemical education.

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[27] A. Das *et al.*,'Hydrocarbons Parser', *minerazzi.com* (Aug 2015), http://www.minerazzi.com/tools/hydrocarbons/parser.php.

CHAPTER 12

INNOVATIVE MNEMONICS FOR THE IUPAC NOMENCLATURE OF BICYCLO AND SPIRO COMPOUNDS

In this last chapter, the IUPAC nomenclature of bicyclo and spiro compounds will be discussed. This is of vital importance for students of organic chemistry from undergraduate to postgraduate levels. These innovative nmemonics have been introduced to determine the IUPAC nomenclature of bicyclo and spiro compounds in a very simple, organic, and time efficient way.

The conventional methods that are generally used to determine the IUPAC nomenclature of bicyclo and spiro compounds are time consuming.[28] With this in mind, two innovative mnemonics have been introduced to determine the IUPAC nomenclature of bicyclo and spiro compounds in a very simple way.[29]

METHODOLOGY

A. Innovative Mnemonics for the IUPAC Nomenclature of Bicyclo Compounds

In bicyclo compounds, two rings are fused with each other and they will have at least 2 common points. These common points (cp), may also be treated as carbons, which are also common in two fused rings. The format of the IUPAC nomenclature for bicyclo compounds is "bicycle [a, b, c] alkane", where "a" and "b" are the maximum and minimum number of points in the fused ring system. This excludes the common points and the

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[28] I. L. Finar, *Organic Chemistry* 1 (Pearson, 6th ed.: 2004), 532; R. T. Morrison *et al.*, *Organic Chemistry* (Pearson, 7th ed.: 2011), 208; T. W. Graham Solomons and C. B. Fryhle, *Organic Chemistry* (Wiley India, 10th ed.: 2012), 150.

[29] A. Das, "Review of Innovative Mnemonics for Inorganic and Organic Chemical Education", *Chemistry Journal* 4 (July 2018): 11 31, http://www.publicscienceframework.org/journal/paperInfo/cj?paperId=3979.

variable “c” = no of common points (cp) – 2.

B. Innovative Mnemonics for the IUPAC Nomenclature of Spiro Compounds

In spiro compounds, two rings pass through one point (intersecting point = 1), which is then elected as the common point. There is always only one common point (cp). It is fish like structure. The format of the IUPAC nomenclature for spiro compounds is “spiro [a, b] alkane”, where “a” and “b” are the minimum and maximum number of points in the fused ring system; this excludes the common point (cp).

RESULTS AND DISCUSSION

A. Innovative Mnemonics for the IUPAC Nomenclature of Bicyclo Compounds

The format of the IUPAC nomenclature for non-substituted bicyclo compounds format is “bicyclo [a, b, c] alkane” and for substituted bicyclo compounds formats it is “x-substituent bicyclo [a, b, c] alkane” with one substituent; “x-substituent bicyclo [a, b, c] alkene/alk-y-ene” with one double bond and one substituent; “x, x-disubstituent bicyclo [a, b, c] alkene/alk-y-ene” with one double bond and two same substituents; and “x, x-disubstituent bicyclo [a, b, c] alka-y, z-diene” with two double bonds and two substituents.

Here, “a” and “b” are the maximum and minimum number of points in the fused ring system; this excludes common points and the variable “c” = number of common points (cp) – 2; x = position number of the substituents present in the ring system; y and z = position numbers of the double bonds and the suffix “alkane”, which corresponds to the total number of points (or carbons) in the fused ring system including common points (bridging points).

Due to the fact that “bicyclo” starts with the letter “b” and “b” stands for “big” (maximum), during the IUPAC nomenclature of bicyclo compounds, first write in the third parenthesis “[ ]”, the maximum number of points followed by the minimum number of points, and then the variable “c” can be found by deducting 2 from the total number of common points [i.e. variable c = number of common points (cp) – 2]. Sometimes, where a = b, then write “a” after “b” or vice versa.

In bicyclo [4, 1, 0] heptanes (Fig. 12.30), the maximum number of points (“a” = 4) is denoted by an asterisk mark. The minimum number (“b”=1”) is denoted by a positive sign, and common points (cp = 2) are denoted by a shadow circle. Adequate examples for the nomenclature of non-substituted bicyclo compounds are given in Fig. 12.31. For substituted bicyclo compounds (Fig. 12.32), the numbering should be started from the common point vertex and continued to the next longest fused ring. This means that the shortest fused ring is numbered last.

B. Innovative Mnemonics for the IUPAC Nomenclature of Spiro Compounds

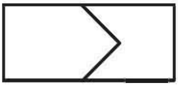
The format of the IUPAC nomenclature for non-substituted spiro compounds is “spiro [a, b] alkane” and for substituted spiro compounds the format is “x-substiuent spiro [a, b] alkane” with one substituent; “x-substituent spiro [a, b] alkene/alk-y-ene” with one double bond and one substituent; “x, x-disubstituent spiro [a, b] alkene/alk-y-ene” with one double bond and two same substituents; and “x, x-disubstituent spiro [a, b] alka-y, z-diene” with two double bonds and two substituents.

Here, “a” and “b” are the minimum and maximum number of points in the fused ring system, excluding the common point (cp); x = position number of the substituents present in the ring system; y and z = position numbers of the double bonds; and the suffix “alkane” corresponds to the total number of points (e.g. the carbon atoms in the ring system including common points).

Due to the fact that in “spiro”, the first letter “s” stands for “small” (minimum), during the IUPAC naming of spiro compounds first write in the third parenthesis “[ ]” the minimum number of points “a” followed by the maximum number of points “b”. Sometimes, where a = b, write “a” after “b” or vice versa. When numbering substituted spiro compounds, give priority to the smaller ring system and start the numbering from the atom next to the common point (cp) and proceed to the smaller ring first and then the bigger ring later on (Fig. 12.33).

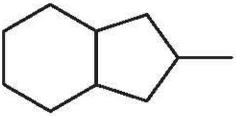
In spiro [2, 4] heptane (Fig. 12.33), the minimum number of points (a = 2) and the maximum number of points (b = 4) is denoted by an arrow mark and the common point (cp = 1) is denoted by an asterisk mark. Adequate examples for the nomenclature of non-substituted and substituted spiro compounds are given in Figures 12.34 and 12.35 respectively.

QUESTIONS ON THE IUPAC NOMENCLATURE OF BICYCLO AND SPIRO COMPOUNDS

Q.1. The compound  is known as:

a. bicyclo [2, 2, 1] heptane b. bicyclo [2, 2, 0] hexane c. bicyclo [2, 2, 0] heptane d. bicyclo [2, 1, 0] heptane

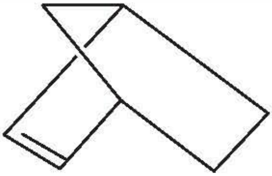
Ans: a. bicyclo [2. 2. 1] heptane

Q.2. The compound  is known as:

a. 1-methylbicyclo [4, 3, 0] nonane b. 8-methylbicyclo [4, 3, 0] nonane c. 3-methylbicyclo [4, 3, 0] nonane d. 4-methylbicyclo [4, 3, 0] nonane

Ans: b. 8-methylbicyclo [4, 3, 0] nonane

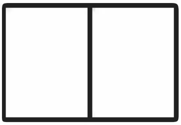
Q.3. The following is a bicyclo [x, y, z] hept-2-ene



where (x+y+z) is

a. 4 b. 3 c. 5 d. 6

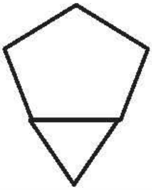
Ans: c. bicyclo [2, 2, 1] hept-2-ene, where x = y = 2 & y = 1; hence, x+y+z = 5



Q.4. The compound, is known as:

a. bicyclo [2, 2, 2] hexane b. bicyclo [3, 2, 1] hexane c. bicyclo [2, 1, 1] butane d. bicycle [2, 2, 0] hexane

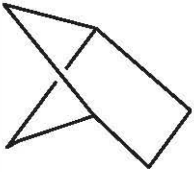
Ans: d. bicyclo [2, 2, 0] hexane



Q.5. The compound, is called:

a. bicyclo [3, 2, 0] hexane b. bicyclo [3, 1,0] hexane c. bicyclo [3, 2, 1] hexane d. bicyclo [2, 2, 0] hexane

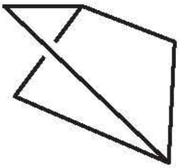
Ans: b. bicyclo [3, 1, 0] hexane



Q.6. The compound, is known as:

a. bicyclo [2, 1, 1] hexane b. bicyclo [2, 2, 0] hexane c. bicyclo [3, 1, 1] hexane d. bicyclo [3, 1, 0] hexane

Ans: a. bicyclo [2, 1, 1] hexane



Q.7. The compound, is known as:

a. bicyclo [2, 1, 0] pentane b. bicyclo [1, 1, 1] pentane c. bicyclo [1, 1, 1] pentane d. bicyclo [2, 1, 1] hexane

Ans: b. bicyclo [1, 1, 1] pentane

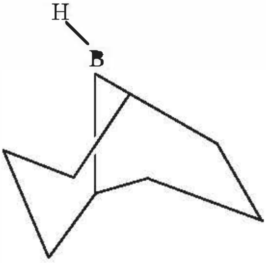
Q.8. The order of priority of the functional groups in the IUPAC system of nomenclature is (STGT 2017):

(a) — CHO > >C=O > —OH > >C=C< (b) >C=O > —CHO > —OH > >C=C<

(c) —CHO > —OH > >C=O > >C=C< (d) >C=C< > —CHO > >C=O > —OH

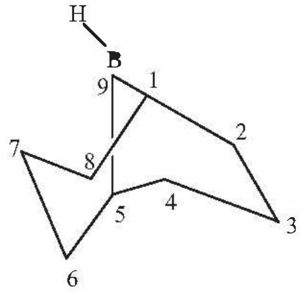
Ans: a) — CHO > >C=O > —OH > >C=C< (see appendix H)

Q.9. The IUPAC name for the following compound is (NET 2017):



a) 9-borabicyclo [3, 3,1] nonane b)1-borabicyclo [3, 3, 1] nonane c) 9-borabicyclo [3, 3,0] octane d)1-borabicyclo [3, 3,0] octane

Ans: a) 9-borabicyclo [3, 3, 1] nonane (where X = Y = CP = 3)



It can be expected that these time efficient organic innovative mnemonics to determine the IUPAC nomenclature of bicyclo and spiro compounds, will help chemistry students from undergraduate to postgraduate level. Experiments, *in vitro*, on 100 students showed that by using these formulae, students could save up to 2–3 minutes in the examination hall. On the basis of this, I can strongly recommend using these time efficient innovative nmemonics to detect hydrocarbons in organic chemistry.

APPENDICES

A: Outermost electrons of Periodic Elements

In case of determination of the hybridization state by innovative mnemonics described in chapter 1, one must have a clear idea about the outermost electrons of different family members in the periodic table as follows:

Family	**Outermost electrons**
Carbon family	04
Nitrogen family	05
Oxygen family	06
Halogen family	07
Inert gas family	08

B: Common electronegative values of elements

In case of determination of different physical and chemical properties by innovative nmemonics described in this book, one must have a clear idea about some common electronegativity values of different periodic elements as follows:

Elements	**Electronegative value**
H & P	1.0
C, S, I	2.5
N, Cl	3.0
O	3.5
F	4.0
Na	1.1
Mg	1.2
Cs	0.7
Se	2.4
Br	2.8
Li	1.0
Be	1.5
B	2.0

Periodic Trends of Electronegativity

Period wise movement (Left to Right) → Electronegativity increases

Group-wise movement (Top to Bottom) → Electronegativity decreases

C: Abbreviations

MA = Monovalent atoms

LP = Lone Pair electrons,

BP = Bond Pair electrons

SLP = σ bonds Lone Pair electrons

DLP = Delocalized Lone Pair

LLP = Localized Lone Pair

DNC = Delocalized Negative Charge

LNC = Localized Negative Charge

SLNC = σ bonds Localized Negative Charge

SLLP = σ bonds Localized Lone Pair electrons

M.O.T. = Molecular Orbital Theory

B.O. = Bond Order

NEET = National Eligibility cum Entrance Test

JEE MAIN = Joint Entrance Examination (engineering entrance examination in India)

STPGT = Selection Test for Post Graduate Teacher

STGT = Selection Test for Graduate Teacher

AIEEE = All India Engineering Entrance Examination

NET = National Eligibility Test (for lectureship and junior research fellowship conducts by the UGC-CSIR)

BMO = Bonding Molecular Orbital

AMBO = Anti Bonding Molecular Orbital

BM = Bohr-Magneton

ND = Next digit

PD = Penultimate digit

IUPAC = International Union of Pure and Applied Chemistry

E.N. = Electronegativity

MCQs = Multiple Choice Questions

CBL = Computer Based Learning

CFT = Crystal Field Theory

LS = Low Spin

HS = High Spin

E.C. = Electronic Configuration

CP = Common Point

DoU = Degree of Unsaturation

D: Correlation between literature values of bond dissociation energy and predicted bond order values

Diatomic species	Bond order Values	Bond dissociation energy (KJ/Mol)
O_2^+	2.5	642.9
O_2	2.0	493.6
O_2^-	1.5	395.0
NO^+	3.0	1046.9
NO	2.5	826.9
NO^-	2.0	487.8
F_2	1.0	157.0
O_2	2.0	498.0
N_2	3.0	945.0

E: Oxoacids and their anions (radicals)

Formula of Oxoacid	Name	Radicals
$HClO_4$	Perchloric acid	tetraoxochlorate (ClO_4^-)
$HClO_3$	Chloric acid	trioxochlorate (ClO_3^-)
$HClO_2$	Chlorous acid	dioxochlorate (ClO_2^-)
$HClO$	Hypochlorous acid	monooxochlorate (ClO^-)
H_3AsO_4	Arsenic acid	tetraoxoarsenate (AsO_4^{3-})
H_3AsO_3	Arsenous acid	trioxoarsenate (AsO_3^{3-})
H_2SO_4	Sulfuric acid	tetraoxosulfate (SO_4^{2-})
H_2SO_3	Sulfurous acid	trioxosulfate (SO_3^{2-})
H_3PO_4	Phosphoric acid	tetraoxophosphate (PO_4^{3-})
H_3PO_3	Phosphorous acid	trioxophosphate (PO_3^{3-})
H_3BO_3	Boric acid	trioxoborate (BO_3^{3-})
H_2CO_3	Carbonic acid	trioxocarbonate (CO_3^{2-})

F: Spin multiplicity and spin State

Number of Unpaired electrons (n)	Spin multiplicity value	Spin State
1	2	Doublet
2	3	Triplet
3	4	Quartet
4	5	Quintet
5	6	Sextet
> 5	> 6	Multiplet

G: IUPAC word root for a number of carbon atoms

No. of Carbons	IUPAC Word root
1C	methane
2C	ethane
3C	propane
4C	butane
5C	pentane
6C	hexane
7C	heptanes
8C	octane
9C	nonane
10C	decane
11C	undecane
12C	dodecane
13C	tridecane
14C	tetradecane
15C	pentadecane
16C	hexadecane
17C	heptadecane
18C	octadecane
19C	nonadecane
20C	eicosa
21C	uneicosa

22C	bieicosa
23C	trieicosa
25C	penteicosa
26C	hexeicosa
29C	noneicosa
30C	tricont
31C	untricont
32C	bitricont
34C	tetratricont
35C	pentatricont
39C	nonatricont
40C	tetracont
44C	tetratetracont
46C	hextetracont
49C	nontetracont
50C	pentacont
60C	hexacont
70C	heptacont
80C	octacont

H: IUPAC suffix and prefix for functional groups

Group	Structure	Prefix	Suffix
Acid	$-COOH$	carboxy	carboxylic or –oic acid
Acid amide	$-CONH_2$	carbamoyl	amide or carboxamide
Acid halide	$-COX$	halocarbonyl	oyl or carbonyl halide
Alcohol	$-OH$	hydroxyl	ol
Aldehyde	$-CHO$	formyl, aldo	al
Amine	$-NH_2$	amino	amine
Carbonitric (nitrile)	$-CN$	cyano	carbonitrile (nitrile)
Double bond	$>C=C<$	-	ene
Ester	$-COO(R)$	alk(yl) oxycarbonyl	carboxylate, oate
Ether	$-O-R$	alkoxy	-
Halide	$-X$	halo	-
Ketone	$R_2C=0$	oxo, keto	one
Sulfonic derivative	$-SO_3H$	sulfo	sulfonic acid
Mercaptan	$-SH$	sulfanyl	thiol
Triple bond	$-C\equiv C-$	-	yne
Anhydride	$-(CO)_2O$	acetoxy or acetyloxy	oic anhydride

Usual order for choosing the principal functional group is given below:

Carboxylic > Sulfonic > acid halide > ester > acid amide > aldehyde > cyanide (nitrile) > isocyanide > ketone > alocohol > phenol > thioalcohol > amine > alkene > alkyne

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FIGURES

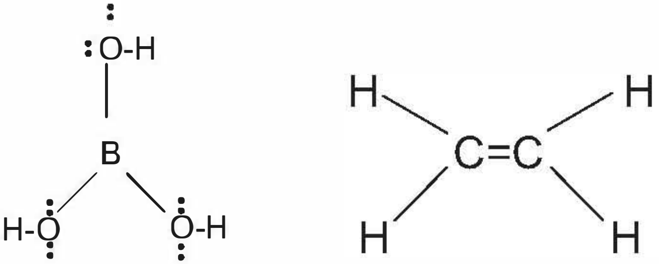


Fig. 1.1 Structure of H_3BO_3 and C_2H_4

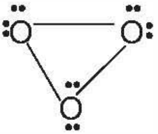


Fig. 1.2 Equilateral triangle structure of cyclic ozone (O_3)

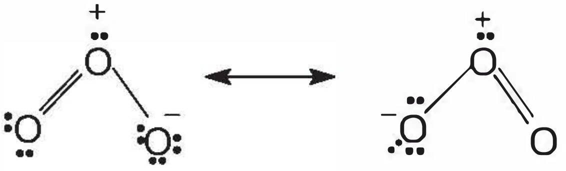


Fig. 1.3 Resonating structures of Ozone (O_3)

(S_8) (P_4)

Fig. 1.4 Zigzag structure of S_8 and Tetrahedron structure of P_4

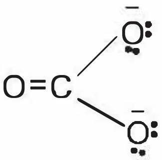


Fig. 1.5 Valence bond structure of carbonate ion (CO_3^{2-})

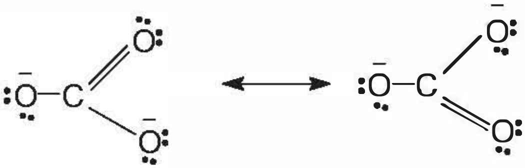


Fig. 1.6 Resonance hybrid of CO_3^{2-}

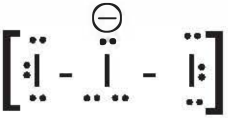


Fig. 1.7 Linear structure of triiodide ion (I_3^-)

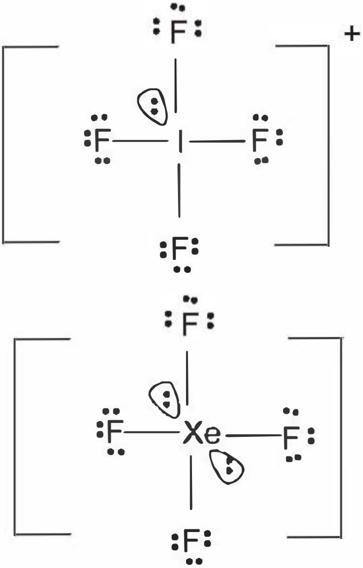


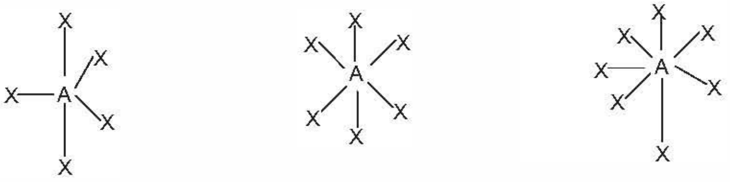
Fig. 1.8 Structure of IF_4^+ and XeF_4

X-A-X

(Linear, sp, LP=0)

(Trigonal planar, sp^2 , LP=0)

(Tetrahedral, sp^3,LP=0)

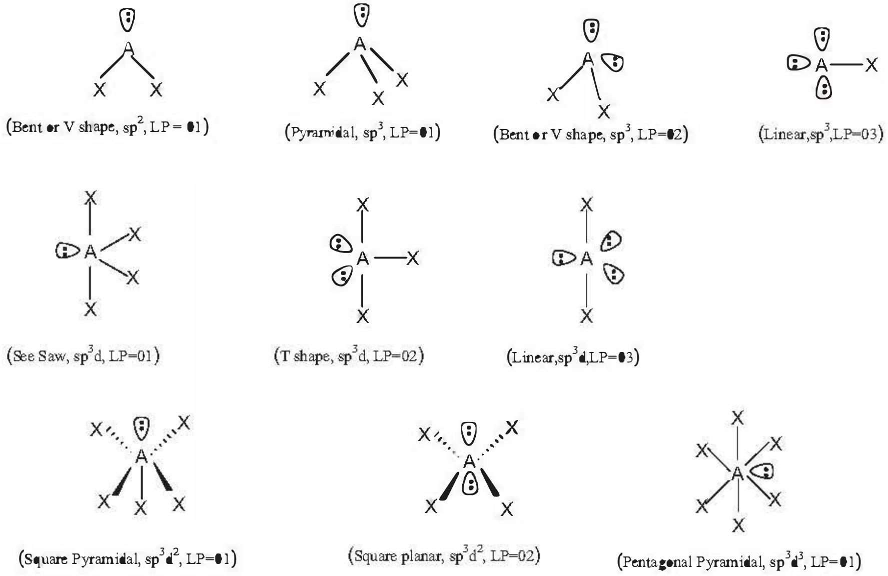


(Trigonal bipyramidal, sp^{3}d, LP=0)

(Octahedral, sp^{3}d^2, LP=0)

(Petntagonal bipyramidal,sp^{3}d^3,LP =0)

Fig.1.9 Regular / Normal Molecular Geometry without Lone pair of electrons

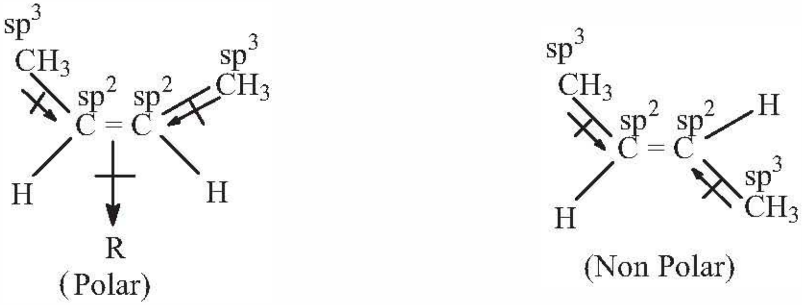


(Bent or V shape, sp^2, LP = 01) (Pyramidal, sp^3, LP=01) (Bent or V shape, sp^3, LP=02) (Linear,sp^3,LP=03)

(See Saw, sp^{3}d, LP=01) (T shape, sp^{3}d, LP=02) (Linear,sp^{3}d,LP=03)

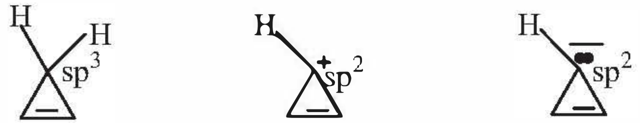
(Square Pyramidal, sp^{3}d^2, LP=01) (Square planar, sp^{3}d^2, LP=02) (Pentagonal Pyramidal, sp^{3}d^3, LP=01)

Fig. 1.10 Sub-normal Molecular Geometry with Lone pair of electrons



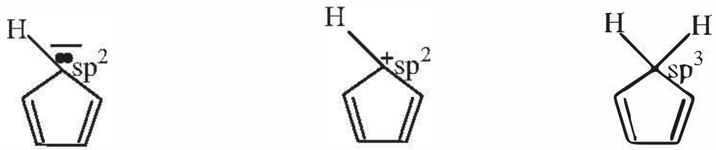
(cis-2-butene, dipole moment μ ≠ 0 D) (trans-2-butene, dipole moment μ = 0 D)

Fig. 1.11: Structure of cis-2-butene and trans-2-butene



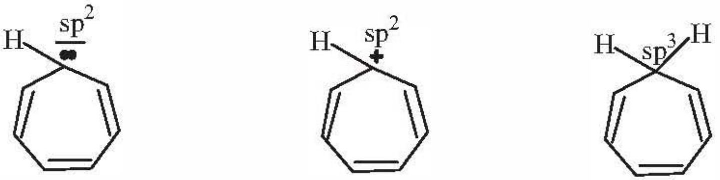
(Cyclopropene) (Cyclopropenyl cation) (Cyclopropenyl anion)

Fig. 2.12: Structure of Cyclopropene, Cyclopropenyl cation, and Cyclopropenyl anion



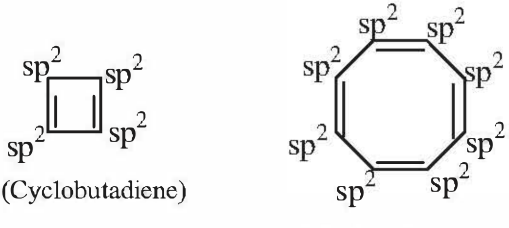
(Cyclopentadienyl anion) (Cyclopentadienyl cation) (Cyclopentadiene)

Fig. 2.13: Structure of Cyclopentadienyl anion, Cyclopentadienyl cation, and Cyclopentadiene



(Cycloheptatrienyl anion) (Cycloheptatrienyl cation) (Cycloheptatriene)

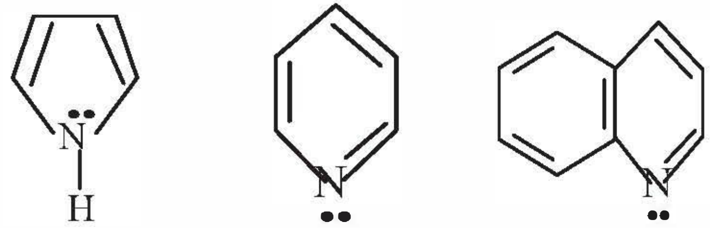
Fig. 2.14: Structure of Cycloheptatrienyl anion, Cycloheptatrienyl cation, and Cycloheptatriene



(Cyclobutadiene)

(Cyclooctatetraene)

Fig. 2.15: Structure of Cyclobutadiene and Cyclooctatetraene



Pyrrole Pyridine Quinoline

Fig. 2.16: Structure of pyrrole, pyridine, and quinoline

Aziridine Oxetan

Fig.2.17: Structure of aziridine and oxetan

$H\text{-}C{\equiv}C\text{-}H$

spsp

Fig. 3.18: Linear structure of Ethyne (C_2H_2)

1 2 3 4 5

$CH_2 = CH \quad CH_2 \quad C \equiv CH$

Fig. 3.19: Structure of pent-1-ene-4-yne

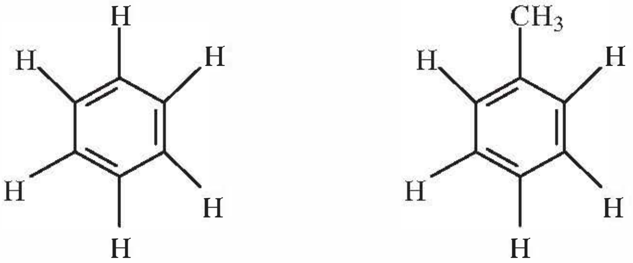


Fig. 3.20 Structure of Benzene and Toluene

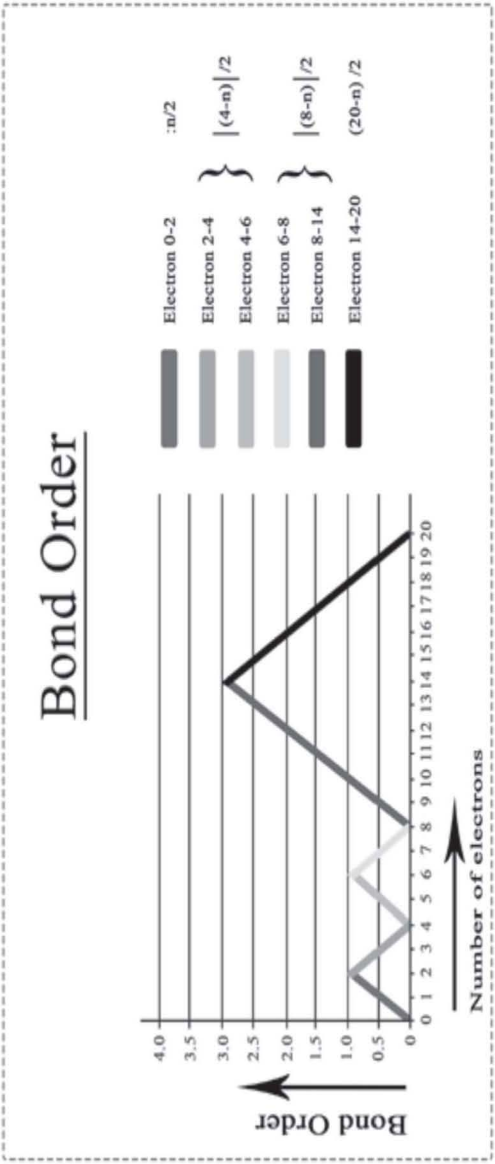
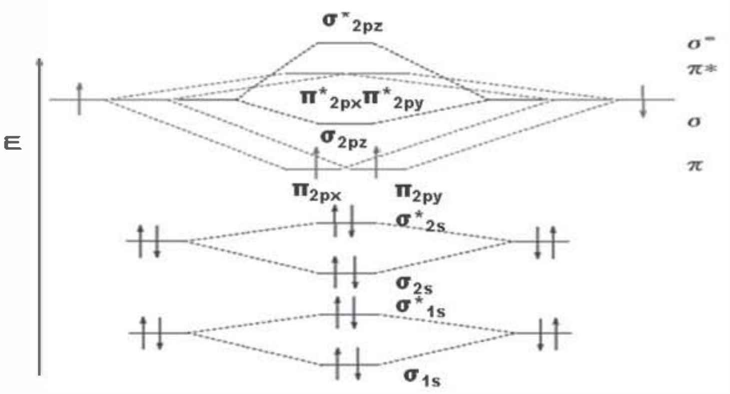


Fig.4.21: Graphical Representation of B.O. with the number of electrons

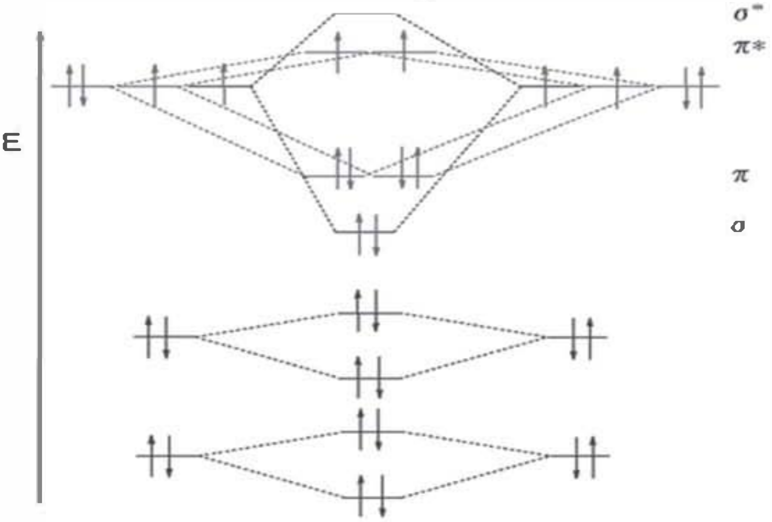
Molecular Orbital Diagram of B_2 having electrons < 14



Bond order of B_2 = without star orbital (BMO) - with star orbital (ABMO) /2 = 6-4/2

Fig.4.22: Molecular orbital diagram of B_2

Molecular Orbital Diagram of O_2 > 14 e^-s



Bond order = $N_{BMO} - N_{ABMO} / 2 = 10 - 6 / 2 = 4/2 = 2$ (O = O)

Fig.4.23: Molecular orbital diagram of O_2

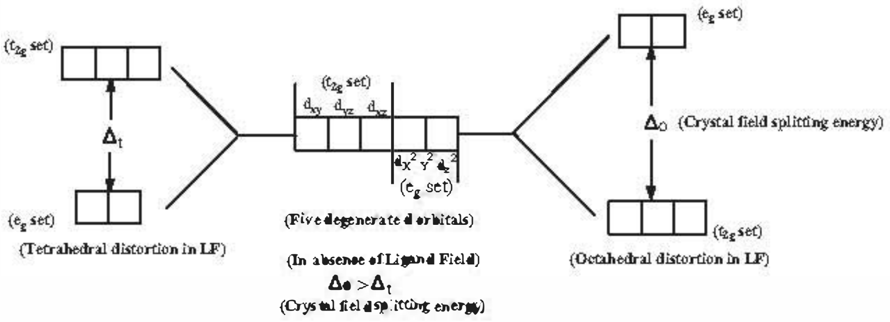
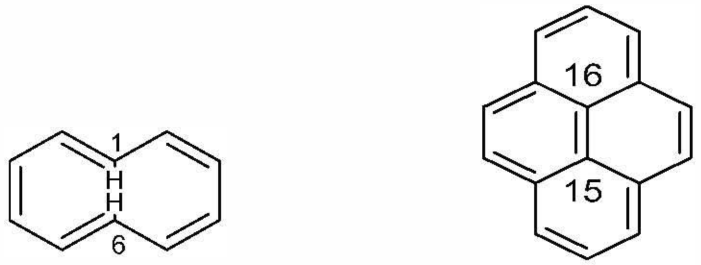


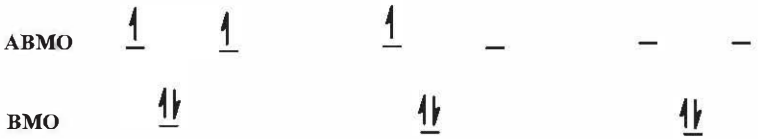
Fig.7.24: Splitting of d orbitals in Crystal Field Theory (CFT)



Cyclodecapentaene

Pyrene

Fig. 8.25.Geometry of Cyclodecapentaene and Pyrene



(Cyclopropenyl anion)

Filled BMO = 1

e^-s in ABMO = 2

(Cyclopropenyl radical)

Filled BMO = 1

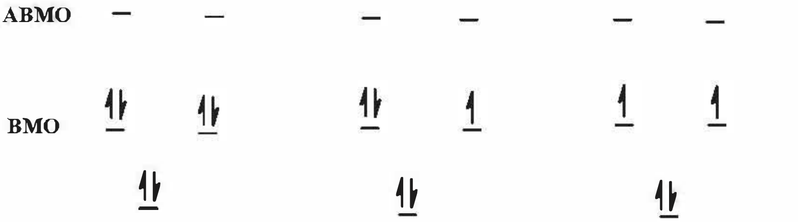
e^-s in ABMO = 1

(Cyclopropenyl cation)

Filled BMO = 1

e^-s in ABMO = 0

Fig.8.26: Molecular orbital diagram of the cyclopropenyl anion, cyclopropenyl radical and cyclopropenyl cation

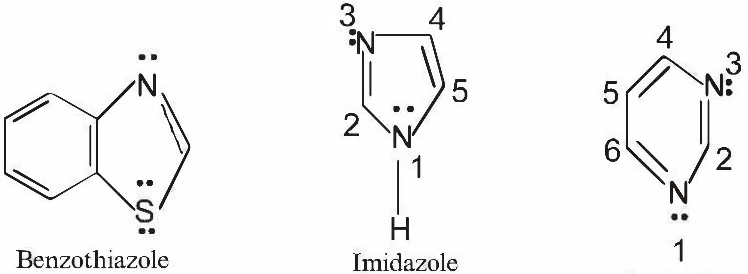


(Cyclopentadienyl anion)
Filled BMOs = 3
e⁻s in ABMO = 0

(Cyclopentadienyl radical)
Filled BMOs = 2
e⁻s in ABMO = 0

(Cyclopentadienyl cation)
Filled BMO = 1
e⁻s in ABMO = 0

Fig.8.27: Molecular orbital diagram of cyclopentadienyl anion, cyclopentadienyl radical and cyclopentadienyl cation

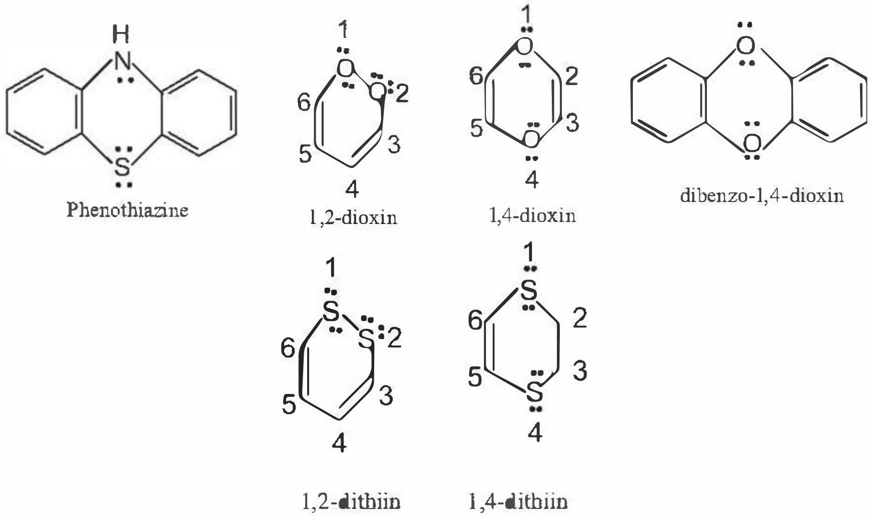


Benzothiazole

Imidazole

Pyrimidine

Fig. 9.28. Structure of Benzothiazole, Imidazole, and Pyrimidine



Phenothiazine

1,2-dioxin

1,4-dioxin

dibenzo-1,4-dioxin

1,2-dithiin

1,4-dithiin

Fig.9.29. Structure of phenothiazine, 1,2-dioxin, 1,4-dioxin, dibenzo-1.4-dioxin and 1,2-dithiin and 1,4-dithiin

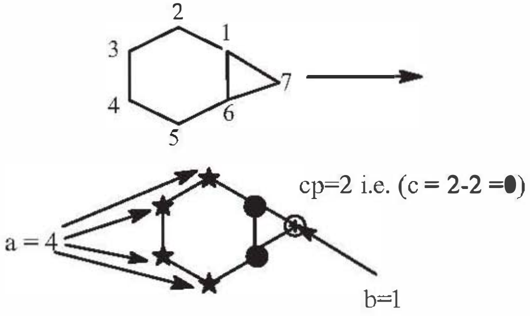


Fig. 12.30. Bicyclo [4,1,0]heptane.

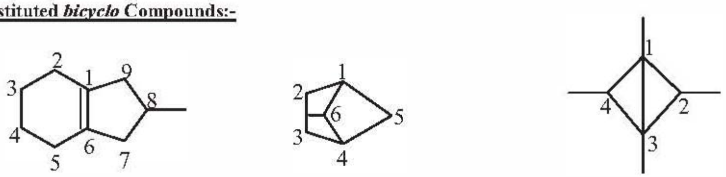
Non substituted *bicyclo* compounds:

bicyclo[2,1,0]pentane bicyclo[3,1,0]hexane bicyclo[3,2,0]heptane bicyclo[2,2,0]hexane

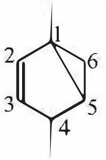
bicyclo[4,1,0]heptane bicyclo[2,2,1]heptane bicyclo[2,2,2]octane bicyclo[4,4,0]decane

Fig. 12.31. IUPAC Nomenclature of non substituted bicyclo compounds.

Substituted *bicyclo* Compounds:-



8-methylbicyclo[4,3,0]nonene 6-methylbicyclo[2,1,1]hexane 1,2,3,4-tetramethylbicyclo[1,1,0]butane



1,4-dimethylbicyclo[3,1,0]hex-2-ene.

Fig. 12.32. IUPAC Nomenclature of substituted bicyclo compounds.

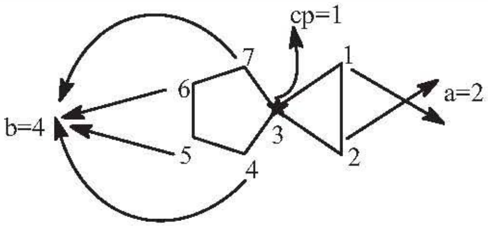
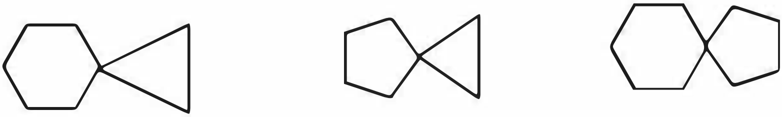


Fig. 12.33. Spiro [2, 4]heptane.

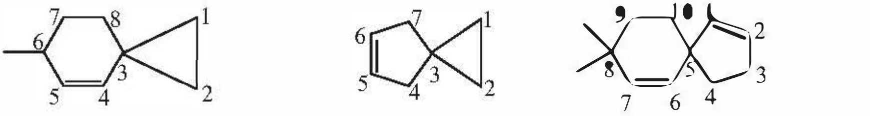
Non Substituted *Spiro* compounds:-



Spiro[2,5]octane Spiro[2,4]heptane Spiro[4,5]decane

Fig. 12.34. Nomenclature of non substituted spiro compounds.

Substituted *Spiro* compounds:-



6-methylspiro[2,5]oct-4-ene Spiro[2,4]hept-5-ene 8,8-dimethylspiro[4,5]deca-1,6-diene

Fig. 12.35. Nomenclature of substituted spiro compounds.

TABLES

Table 1.1 T_{SLP} and corresponding hybridization state

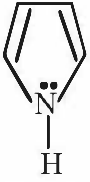
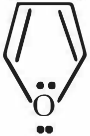
T_{SLP} (Total number of σ bonds + LP)	Nature of Hybridization State	Examples
2	sp	$BeCl_2$, $HgCl_2$,C_2H_2,$C●_2$,$C●$,$CdCl_2$, $ZnCl_2$ etc.
3	sp^2	BCl_3, $AlCl_3$,C_2H_4,C_6H_6,$S●_2$,$S●_3$,$HN●_3$, $H_2C●_3$,$SnCl_2$, $PbCl_2$ etc.
4	sp^3	NH_4^+, BF_4^-, $H_2S●_4$, $HCl●_4$,PCl_3, NCl_3, $AsCl_3$, $HCl●_3$,ICl_2^+,$●F_2$,$HCl●_2$,SCl_2,$HCl●$, ICl, $Xe●_3$ etc.
5	sp^3d	PCl_5, $SbCl_5$, SF_4, ClF_3, BrF_3, XeF_2, ICl_2^- etc.
6	sp^3d^2	SF_6, AlF_6^{3-}, SiF_6^{2-}, PF_6^-, IF_5, BrF_5, $Xe●F_4$, XeF_4, BrF_4^-, ICl_4^- $[TeF_5]^-$ etc.
7	sp^3d^3	IF_7, XeF_6 etc.

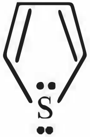
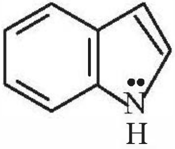
Table 1.2 Hybridization, Molecular Geometry, and Bond Angles

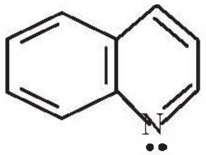
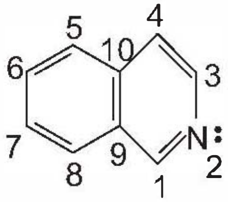
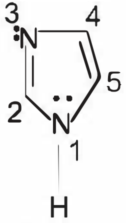
Hybridization	LP	Molecular Geometry (Regular / Normal)	Approximate Bond Angles (Degree)	Examples	LP	Molecular Geometry (Sub-normal)	Approximate Bond Angles (Degree)	Example
sp	0	Linear	180	CO_2, CS_2, $BeCl_2$, $HgCl_2$	-	-	-	-
sp^2	0	Trigonal Planar or Triangular Planar	120	BH_3, $AlCl_3$, C_2H_4, BCl_3, BF_3, NO_3^-, CO_3^{2-}	01	Angular or V-shape	<120	SO_2, NO_2^-
sp^3	0	Tetrahedral	109.5	BH_4^-, BF_4^-, $SnCl_4$, H_2SO_4, $HClO_4$, $SiCl_4$	01	Pyramidal	<109.5	NH_3, PH_3, AsH_3, XeO_3 ClO_3^-
					02	Bent shape or V-shape	<109.5	H_2O, H_2S, H_2Se
					03	Linear	180	ICl, BrF, ClF

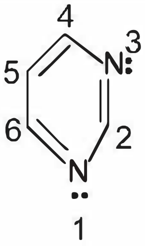
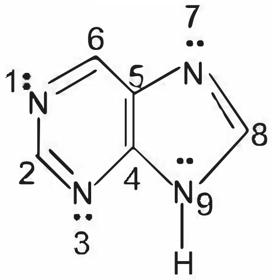
sp^{3}d	0	Trigonal bipyramid	120 (equatorial) 90 (axial)	PF_5, PCl_5	01	See-Saw	<120 (equatorial) <90 (axial)	SF_4
					02	T-shape	<90	ICl_3, F_3Cl
					03	Linear	180	XeF_2, I_3^-
sp^{3}d^2	0	Octahedral	90	SF_6, TeF_6, WF_6, SeF_6, $SnCl_6^{2-}$	01	Square pyramidal	<90	IF_5, BrF_5 $[TeF_5]^-$
					02	Square planar	90	XeF_4
sp^{3}d^3	0	Pentagonal bipyramid	72 & 90	IF_7	01	Pentagonal Pyramidal or Distorted octahedral	72 & 90	XeF_6

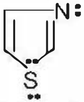
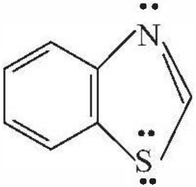
Table-2.3 Hybridization state of Heteroatom in Heterocyclic Compounds with the help of LLP

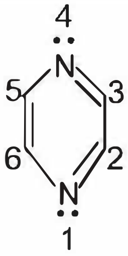
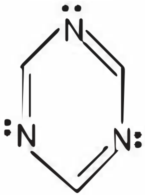
Heterocyclic Compounds (Planar/nonplanar)	Number of σ bonds around the hetero atom (from single and double bonds) (T_S)	Number of localized Lone Pair of e^-s (LLP)	Total Number of σ bonds around the hetero atom (T_{SLLP})	Power on the Hybridization state of the heteroatom **(P_{Hyb}) = (T_{SLLP}) – 1** (Corresponding Hybridization state)
 Pyrrole (Planar)	03	0 (the lone pair of electron undergo delocalization, DLP with the ring system)	03	02 (sp^2 N)
 Furan (Planar)	02	01 (out of two lone pairs of electrons, one undergo delocalization, DLP and other remain as LLP)	03	02 (sp^2 O)

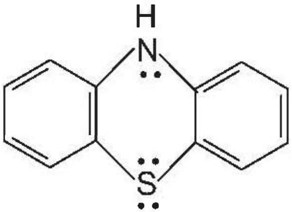
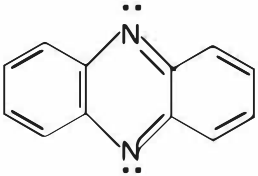
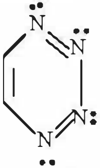
 Thiophene (Planar)	02	01 (out of two lone pairs of electrons of S one undergo delocalization, DLP and other remain as LLP)	03	02 (sp^2 S)
 Pyridine (Planar)	02	01	03	02 (sp^2 N)
 Indole (Planar)	03	0	03	02 (sp^2 N)

 Quinoline (Planar)	●2	●1	●3	●2 (sp^2 N)
 Isoquinoline (Planar)	●2	●1	●3	●2 (sp^2 N)
 Imidazole (Planar)	●3 (N1) ●2 (N3)	● (N1) ●1 (N3)	●3 ●3	●2 (sp^2 N1) ●2 (sp^2 N3)

 Pyrimidine (Planar)	●2 (N1) ●2 (N3)	●1 (N1) ●1 (N3)	●3 ●3	●2 (sp^2 N1) ●2 (sp^2 N3)
 Purine (Planar)	●2 (N1) ●2 (N3) ●2 (N7) ●3 (N9)	●1 (N1) ●1 (N3) ●1 (N7) ● (N9)	●3 ●3 ●3 ●3	●2 (sp^2 N1) ●2 (sp^2 N3) ●2 (sp^2 N7) ●2 (sp^2 N9)

 Thiazole (Planar)	●2 (N) ●2 (S)	●1 (N) ●1 (S) (out of two lone pairs of electrons on S, one undergo delocalization, DLP and other remain as LLP)	●3 ●3	●2 (sp^2 N) ●2 (sp^2 S)
 Benzothiazole (Planar)	●2 (N) ●2 (S)	●1 (N) ●1 (S) (out of two lone pairs of electrons on S, one undergo delocalization, DLP and other remain as LLP)	●3 ●3	●2 (sp^2 N) ●2 (sp^2 S)

 Pyrazine (p-diazine) (Planar)	●2 (N1) ●2 (N1)	●1 (N1) ●1 (N1)	●3 ●3	●2 (sp^2 N1) ●2 (sp^2 N4)
 Cyanidine (Planar)	●2 (N1, N3, and N5)	●1 (N1, N3, and N5)	●3	●2 (sp^2 N1,N3,N5)

 Phenothiazine (Planar)	●3 (N) ●2 (S)	● (N) ●1 (S) (out of two LP of S, one undergo delocalization(DLP), and others remain as LLP)	●3 ●3	●2 (sp^2 N) ●2 (sp^2 S)
 Phenazine (Planar)	●2 (both N)	●1 (both N)	●3	●2 (sp^2 both N)
 1,2,3,4-tetrazine (Planar)	●2 (N1,N2,N3,N4)	●1 (N1,N2,N3,N4)	●3	●2 (sp^2 All N)

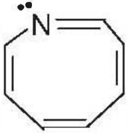
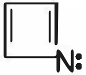
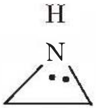
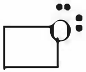
 Azocine (Planar)	●2	●1	●3	●2 (sp^2 N)
 Azetine (Planar)	●2	●1	●3	●2 (sp^2 N)
 Aziridine (non-planar)	●3	●1	●4	●3 (sp^3 N)
 Oxetan (non-planar)	●2	●2	●4	●3 (sp^3 O)

Table 4.4 Bond order of diatomic species having (1-20) electrons

Species (Molecules or ions)	Total Number of e^-s (n)	Bond-Order (B.O.)
Bond-Order Values for the species having (1-2) e^-s; Bond order = n/2		
H_2^+	1	0.5
H_2, He_2^{2+}	2	1
Bond-Order Values for the species having (2-6) e^-s; Bond order = I 4-n I / 2		
H_2^-,He_2^+	3	0.5
He_2,	4	0
Li_2^+,He_2^-	5	0.5
Li_2, He_2^{2-}, Be_2^{2+}	6	1
Bond-Order Values for the species having (6-14) e^-s; Bond order = I 8-n I / 2		
Be_2^+, Li_2^-	7	0.5
Be_2, Li_2^{2-}	8	0
Be_2^-, B_2^+	9	0.5
B_2, Be_2^{2-}, HF	10	1
B_2^-, C_2^+	11	1.5
C_2, B_2^{2-}, N_2^{2+}, CN^+	12	2
C_2^-, N_2^+	13	2.5
N_2, CO, NO^+, C_2^{2-}, CN^-, O_2^{2+}	14	3
Bond-Order Values for the species having (14-20)e^-s ; Bond order = (20-n) / 2		
N_2^-,NO,O_2^+	15	2.5
NO^-, O_2	16	2
O_2^-	17	1.5
F_2, O_2^{2-}, HCl	18	1
F_2^-	19	0.5
Ne_2	20	0

Table 5.5 Magnetic moments (μ_s) in B.M. of diatomic species

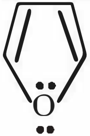
Species (Molecules or ions)	Total Number of e^-s	Number of unpaired electrons (n)	Magnetic moment (μ_s) in Bohr Magneton (B.M.)	Remark on magnetic behavior
H_2^+	1	1	1.73	Para magnetic
H_2, He_2^{2+}	2	0	0	Diamagnetic
H_2^-,He_2^+	3	1	1.73	Para magnetic
He_2,	4	0	0	Diamagnetic
Li_2^+,He_2^-	5	1	1.73	Para magnetic
Li_2, He_2^{2-}, Be_2^{2+}	6	0	0	Diamagnetic
Be_2^+,Li_2^-	7	1	1.73	Para magnetic
Be_2,Li_2^{2-}	8	0	0	Diamagnetic
Be_2^-,B_2^+	9	1	1.73	Para magnetic
B_2, Be_2^{2-},HF	10	2	2.82	Para magnetic
B_2^-,C_2^+	11	1	1.73	Para magnetic
C_2,B_2^{2-},N_2^{2+}, CN^+	12	0	0	Diamagnetic
C_2^-,N_2^+	13	1	1.73	Para magnetic
N_2,CO,NO^+,C_2^{2-},CN^-,O_2^{2+}	14	0	0	Diamagnetic
N_2^-,NO,O_2^+	15	1	1.73	Para magnetic
NO^-,O_2	16	2	2.82	Para magnetic
O_2^-	17	1	1.73	Para magnetic
F_2,O_2^{2-},HCl	18	0	0	Diamagnetic
F_2^-	19	1	1.73	Para magnetic
Ne_2	20	0	0	Diamagnetic

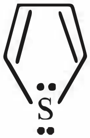
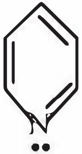
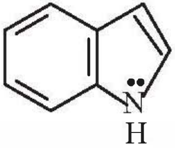
Table 8.6 Aromatic, anti-aromatic and non-aromatic behavior of organic compounds

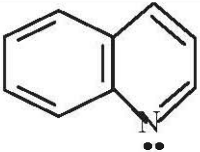
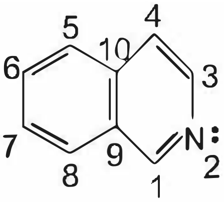
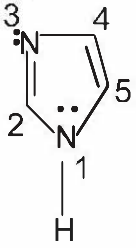
Organic Compound (Cyclic, Planar/Cyclic, non-planar)	πb value [πb =number of π bonds within the ring system]	e^-p value [e^-p = number of delocalized electron pair outside or adjacent to the ring system]	A value [A = πb + e^-p + 1(constant)] (even no/odd no)	Nature of compound (aromatic/anti-aromatic/non 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

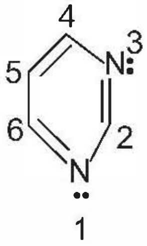
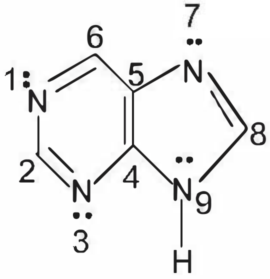
Cyclobutadiene or [4] annulene (Cyclic, Planar)	2 π bonds	●	2 + ● + 1 = 3 (odd no)	Anti aromatic
Cyclopentadiene (Cyclic, non planar due to one sp^3 hybridised carbon atom)	2 π bonds	●	2 + ● + 1 = 3 (odd no)	Non-aromatic
Cyclopentadienyl cation (Cyclic, Planar)	2 π bonds	●	2 + ● + 1 = 3 (odd no)	Anti-aromatic
Cyclopentadienyl anion (Cyclic, Planar)	2 π bonds	●1(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	●	4 + ● + 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	●	3 + ● + 1 = 4 (even no)	Non aromatic

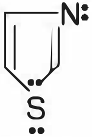
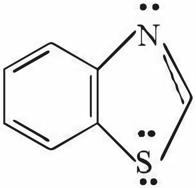
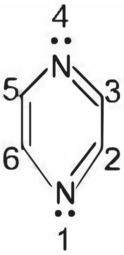
Table 9.7 Aromatic, anti-aromatic, and non-aromatic behavior of heterocyclic compounds

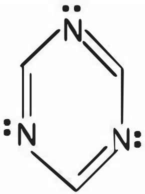
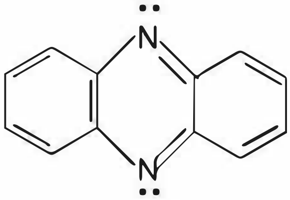
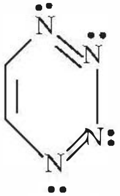
Hetero Cyclic Compound (Cyclic, Planar, Conjugated)	πb value [πb =number of π bonds within the ring system	DLP	A value [A = πb + DLP + 1(constant)] (even No /odd No)	Remark on Nature of compound (Aromatic/Anti Aromatic)
 Pyrrole	2	1	2 + 1 + 1 = 4 (even No)	Aromatic
 Furan	2	1 (Here out of two lone pairs on O only one LP take part in delocalization)	2 + 1 + 1 = 4 (even No)	Aromatic

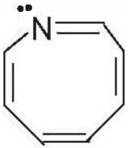
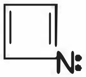
 Thiophene	2	1 (Here out of two lone pairs on ● only one LP take part in delocalization)	2 + 1 + 1 = 4 (even No)	Aromatic
 Pyridine	3	0	3 + 0 + 1 = 4 (even No)	Aromatic
 Indole	4	1	4 + 1 + 1 = 6 (even No)	Aromatic

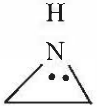
 Quinoline	5	●	5 + ● + 1 = 6 (even No)	Aromatic
 Isoquinoline	●5	●	5 + ● + 1 = 6 (even No)	Aromatic
 Imidazole	●2	●1 (N1)	2 + 1 + 1 = 4 (even No)	Aromatic

 Pyrimidine (m-diazine)	03	0 (N1)	3 + 0 + 1 = 4 (even No)	Aromatic
 Purine	04	01 (N9)	4 + 1 + 1 = 6 (even No)	Aromatic

 Thiazole	●2	●1 (S)	2 + 1 + 1 = 4 (even No)	Aromatic
 Benzothiazole	●4	●1 (S)	4 + 1 + 1 = 6 (even No)	Aromatic
 Pyrazine (p-diazine)	●3	●	3 + ● + 1 = 4 (even No)	Aromatic

 Cyanidine	03	0	3 + 0 + 1 = 4 (even No)	Aromatic
 Phenazine	07	0	7 + 0 + 1 = 8 (even No)	Aromatic
 1,2,3,4-tetrazine	03	0	3 + 0 + 1 = 4 (even No)	Aromatic

 Azocine	04	0	4 + 0 + 1 = 5 (odd No)	Anti aromatic
 Azetine	02	0	2 + 0 + 1 = 3 (odd No)	Anti aromatic

Hetero Cyclic Compound (Cyclic, non-planar)	πb value [πb =number of π bonds within the ring system]	DLP	A value [A = πb + DLP + 1(constant)] (even No/odd No)	Remark on Nature of compound
 Aziridine	-	-	-	Non-Aromatic (nonplanar – sp^3)

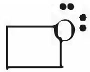
 Oxetan	-	-	-	Non-Aromatic (nonplanar – sp^3)

Table 10.8 Calculation of bonds in open chain olefinic hydrocarbons

Example (C_xH_y)	Straight-chain Structure	π bond/ bonds [(2X-Y)/2+1]	σ bonds [X+Y-1]	Single bonds [(3Y/2)-2]	Double bond/bonds [(2X-Y)/2 + 1]
C_2H_4	$H_2C=CH_2$	1	5	4	1
C_3H_6	$H_2C=CH-CH_3$	1	8	7	1
C_3H_4	$H_2C=C=CH_2$	2	6	4	2
C_4H_8	i)$H_2C=CH-CH_2-CH_3$ ii)$H_3C-HC=CH-CH_3$	1	11	10	1

C_4H_6	i)$H_2C=C=CH-CH_3$ ii)$H_2C=CH-CH=CH_2$	2	9	7	2
C_4H_4	$H_2C=C=C=CH_2$	3	7	4	3
$C_{176}H_{250}$	-	52	425	373	52
$C_{2000}H_{2000}$	-	1001	3999	2998	1001
$C_{99}H_4$	-	98	102	4	98

Table 10.9 Calculation of bonds in Cycloalkene system

Example (C_xH_y)	Cycloalkene	π bond / bonds (P_c) = [(2X-Y)/2]	σ bonds (S_c) [X+Y]	Single bonds (A_c) [(3Y/2)]	Double bond/bonds [(2X-Y)/2]
C_3H_4	Cyclopropene	1	7	6	1
C_4H_4	Cyclobutadiene	2	8	6	2
C_5H_6	Cyclopentadiene	2	11	9	2
C_6H_8	Cyclohexadiene	2	14	12	2
C_7H_8	Cycloheptatriene	3	15	12	3
C_8H_8	Cyclooctatetraene	4	16	12	4

Table 11.10 Calculation of bonds in an open chain alkyne system

Example for Open Chain Alkyne (C_xH_y)	π bonds [{(2X-Y)/2} + 1]	σ bonds [X+Y-1]	Single bonds [{(2X+5Y)/2} - 3]/2	Triple bond/bonds [{(2X-Y)/2} + 1]/2
$C_{10}H_{18}$	2	27	26	1
$C_{11}H_{20}$	2	30	29	1
$C_{12}H_{22}$	2	33	32	1
$C_{13}H_{24}$	2	36	35	1
$C_{14}H_{26}$	2	39	38	1
$C_{15}H_{28}$	2	42	41	1
$C_{16}H_{30}$	2	45	44	1
C_6H_6	4	11	9	2
$C_{12}H_{14}$	6	25	22	3

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