Aromaticity & Bayers Strain Angle Theory

Course on General Organic Chemistry (GOC) for Dropper 13th students

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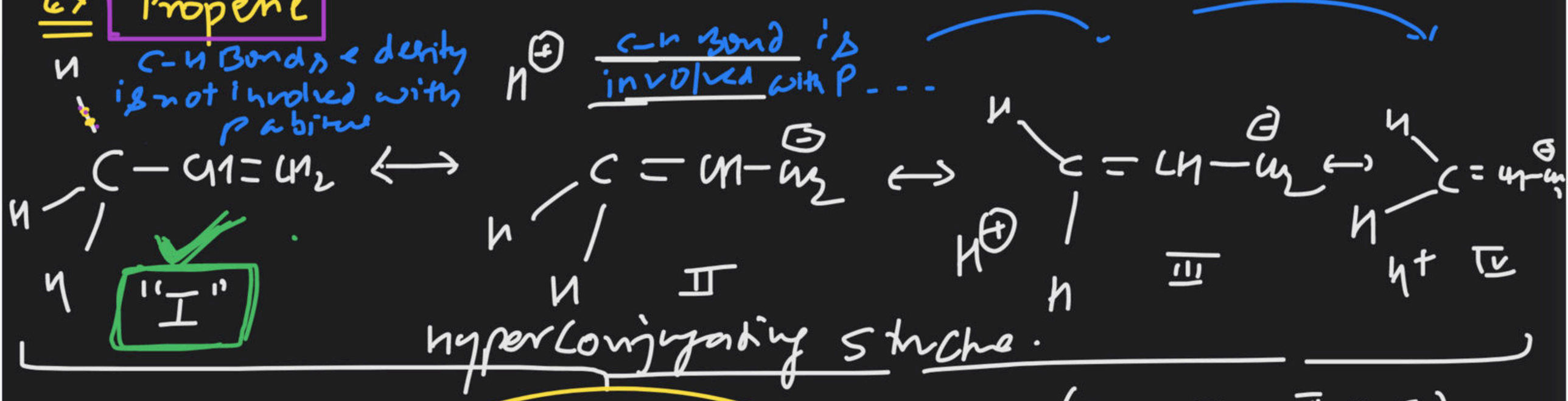
Ex **Propene**

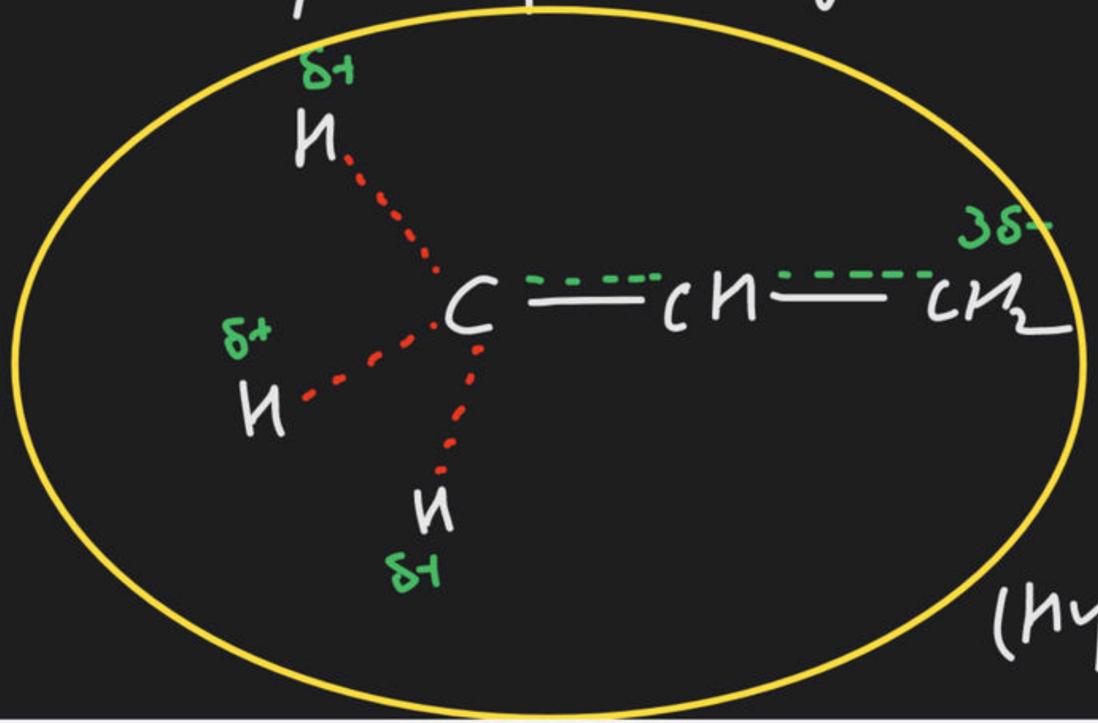
C–H Bonds e density is not involved with p orbital



C–H bond is involved with P - - -

Hyperconjugating structure.

(I > II = III = IV)



(Hyperconjugating Hybrid)

Note: (i) Hyperconjugation effect is also known as Nathan Baker effect.

(ii) Hyperconjugation phenomenon is also known as No Bond Resonance.

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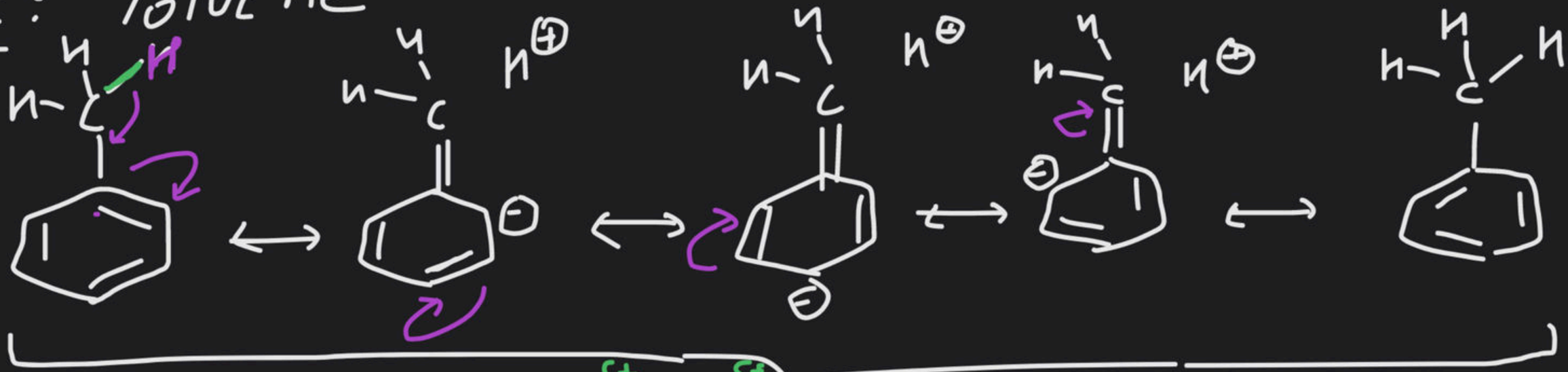
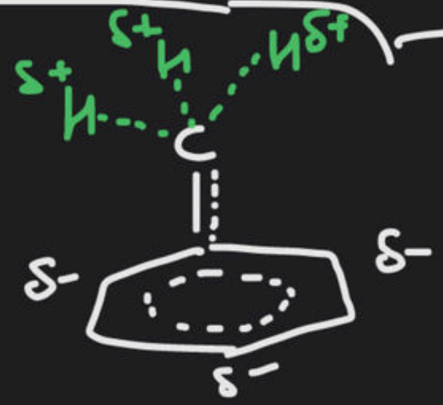
(iii) Total No. of H.S = H.S not involving C–H Bond with p orbital + H.S involving C–H Bond with p orbital

$= 1 + N_{\alpha H}$

Note above formula can be used only when hyperconjugation is the only phenomenon is present in molecule.

Ex: Toluene

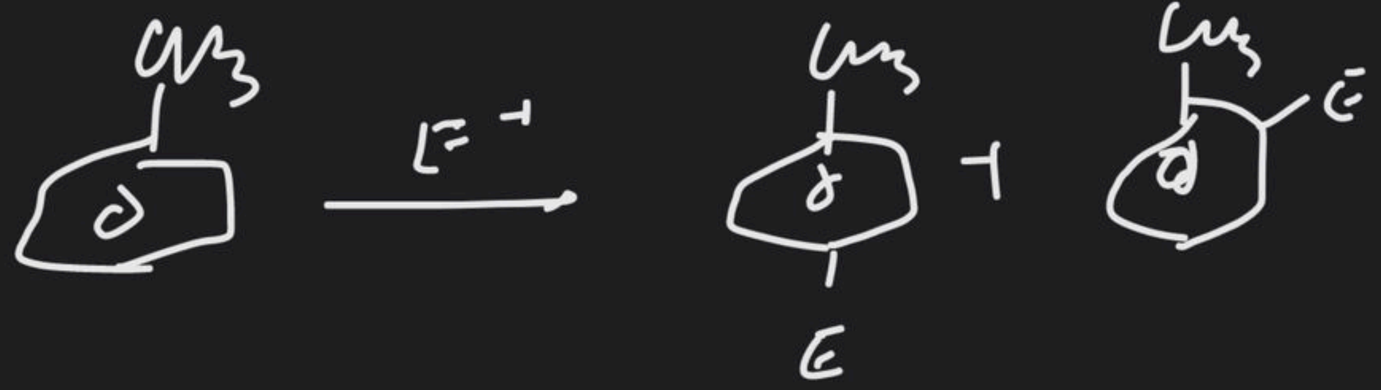




⇒ +H effect is a electron donating effect

⇒ +H effect increses electron density at ortho & para position.

⇒ +H effect is ortho & para directing for incoming electrophile



Ex: Arrange following in ↓ order of +H effect when following groups are connected with π electron system.

(a) $-CH_3$ $-CH_2-CH_3$ $-CH(CH_3)_2$ $-C(CH_3)_3$

1 > 2 > 3 > 4

(b) $-CH_3$ $-CD_3$ $-CT_3$

(c) $-CH_3$, $-CH_2D$, $-CHD_2$, $-CD_3$

(d) $-CH_2-CH_3$ $-CH_2-CH_2-CH_3$

Ex: Identify Intermidiates / Compounds which can show Hyperconjugation phenomenon.

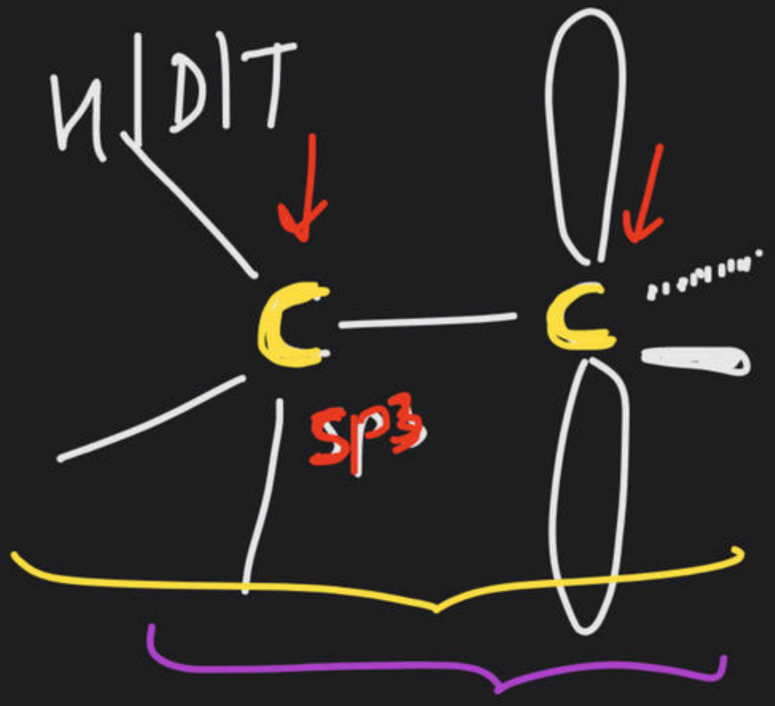
(1) $CH_3^{\oplus}$ NO

(2) $CH_2-CH_3^{\oplus}$

(3) $CH_3-\overset{\oplus}{C}H-CH_3$ yes

(4) $CH_3-CH_2-\overset{\oplus}{C}H_2$

(5) $CH_3-CH(CH_3)-\overset{\oplus}{C}H_2$ yes



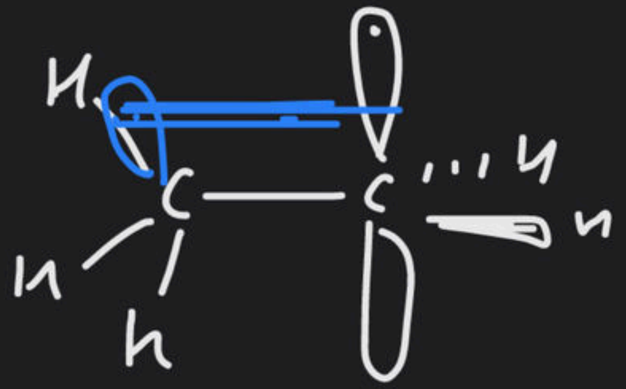
(A) yes
(B) NO

(6) $CH_3-\overset{\ominus}{C}H_2$ (sp3, sp3)

(7) $CH_3-\dot{C}H_2$

(8) $CH_3-CH=CH_2$

(9) $(CH_3)_2C=CH_2$



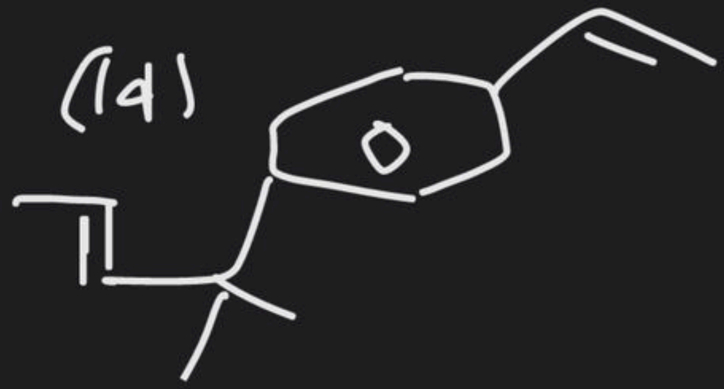
(10)

(11)

(12)

(13)

(14)

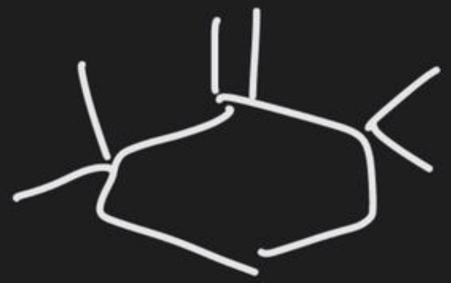


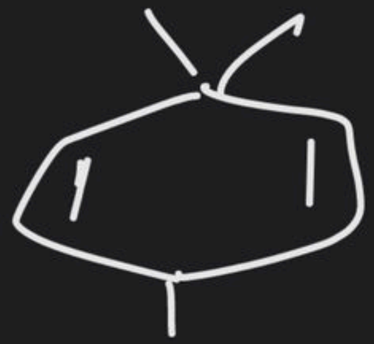
(15) $CH_2=CH-CH_3$

(16) $CH_3-CH=O$

(17) $CH_3-C\equiv CH$

(18) 

(19) 

(20) 

Ex: Total no. of Hs involving C-H Bond of following :-

(a) $CH_3^{\oplus}$ — 0

(b) $CH_3-CH_2^{\oplus}$ — 3

(c) $CH_3-CH_2-CH_2^{\oplus}$ — 2

(d) $CH_3-CH=CH_2$ — 6

H. str

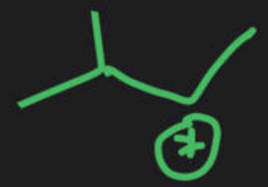
(e) — 6

(f) — 6

(g) — 6

(h) 

(1)

(i) 

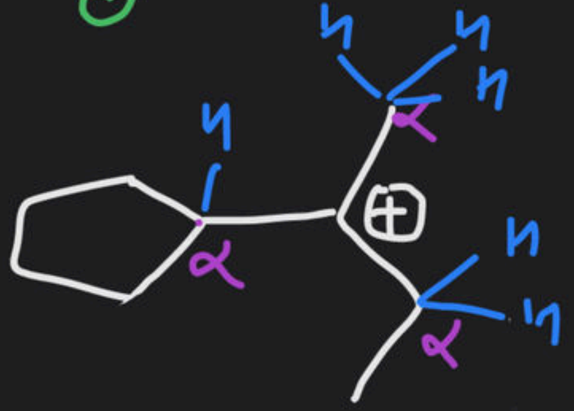
(j) 

I2T

Constructive interfere.

e > g > f

Stability order



(6)

(#) Effectiveness Order of Electronic displacement effects

$$R > M > I$$

Aromaticity

(*)

Bonding orbital $\Longrightarrow$ Aromatic Compounds

Non Bonding orbital $\Longrightarrow$ Non Aromatic Compounds

Anti Bonding orbital $\Rightarrow$ Anti Aromatic Compounds

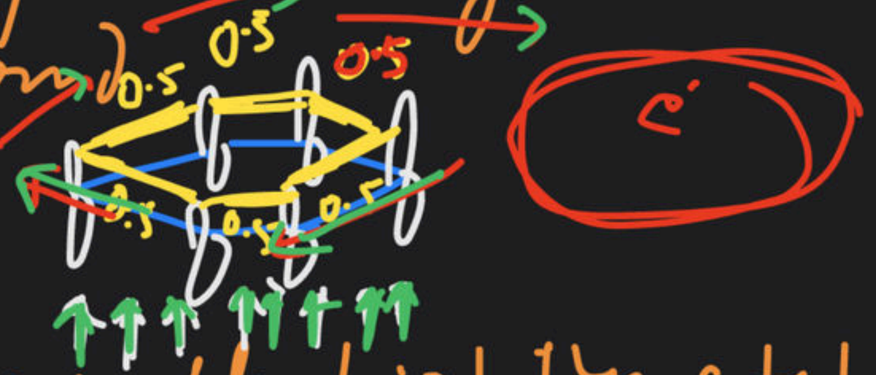
Aromatic Compound

Compounds obtained on fractional distillation of coal tar having a characteristic

Aroma are known as Aromatic compounds.

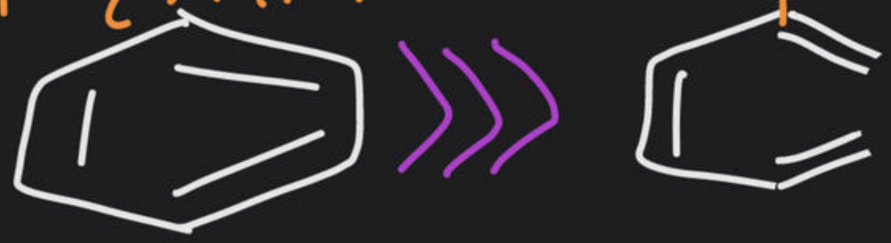
(or)

Compounds having Induced diamagnetic Ring Current are known as Aromatic Compounds



(or)

All cyclic Compounds which are unusually highly stable than its open chain analogues form are known as Aromatic Compounds.



Condition for a Compound to be Aromatic

Compound must

(a) be cyclic

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(b) be planar

(c) be Conjugated (each atom must contain p orbital)

(d) have $(4n+2)$ no. of π electrons (Huckle's Rule)

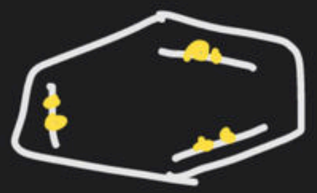
where $(n = 0, 1, 2, 3, 4 \ldots\ldots\ldots)$

(mono cyclic system)

N. No. (2, 6, 10, 14, 18 .....) $\pi e^{\ominus}$s

(Largest Conjugated Periphery).

Ex:



Cyclic ✓
Conjugate ✓
Planer ✓
$\pi e^- s = 6$ ✓

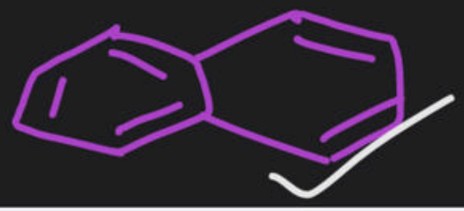
Aromatic

Ex:

Cyclic ✓
Conjugate ✓
Planer ✓
$\pi e^- s = 6$ ✓

Aromatic

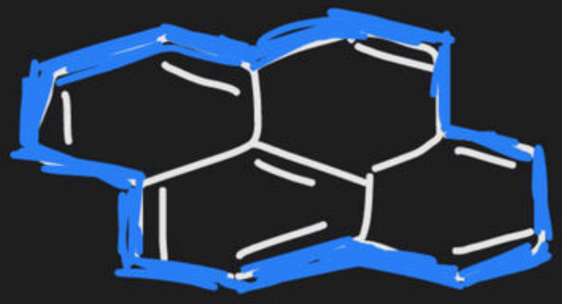
Ex:



Cyclic ✓
Conjugate ✓
Planer ✓
$\pi e^- s = 10$ ✓

Aro

Ex:



Cyclic ✓ ✓
Planer ✓
Conjugate ✓
Peripheral $\pi e^- s = 14\ \pi$ ✓

Aromatic

Ex-1: 1 — 90