Allyl Cl l

The 2 electron cation π system is more stable as a ring. It is an aromatic system.

Thought Experiment

Is a ring more stable (A) or less (B)?

Cyclopropenyl Cation

Cyclopropenyl Anion

The 4 electron anion π system is less stable as a ring. It is an antiaromatic system.

Thought Experiment

Is a ring more stable (A) or less (B)?

C4H4

The 4 electron π system is less stable as a ring. It is an antiaromatic system.

Is a ring more stable (A) or less (B)?

C4H4+2

The 2 electron π system is more stable as a ring. It is an aromatic system.

Is a ring more stable (A) or less (B)?

C6H6

The 6 electron π system is more stable as a ring. It is an aromatic system.

Is a ring more stable (A) or less (B)?
Is a ring more stable (A) or less (B)

Aromatic system
\[ n_e = 6 \]
\[ C_6H_6 \]

Don't form a square, form a rectangle

Is a ring more stable (A) or less (B)

Transition metal stabilized \[ C_6(C_6H_5)_3^+ \]

Co(C_6(C_6H_5)_3)(CO)_3

T. Chiang, R.C. Kerber, S.D. Kimball, J.W. Lauher
*Inorganic Chemistry, 1979, vol 18, page 1687*

Aromatic systems
\[ n_e = 2 \]
\[ C_6H_6^+ \]

Anti-aromatic systems
\[ n_e = 4 \]
\[ C_4H_4 \]

Early studies at Stony Brook 30 years ago by Allen Krantz

\[ 1.52 \text{ Å} \]
\[ 1.44 \text{ Å} \]

Tetra(t-butyl)cyclobutadiene

C_{6}H_{6}^{2-} is also very reactive, but it can be isolated as a salt with large substituents.

\[ 1.49 \text{ Å} \]
\[ 1.49 \text{ Å} \]
Back to diatomics

Homonuclear Diatomic

Bond Order

\[ \begin{align*}
A & : 0 \\
B & : 0.5 \\
C & : 1 \\
D & : 1.5 \\
E & : 2 \\
F & : 2.5 \\
G & : 3
\end{align*} \]

Bond Order = \frac{\text{Bond } e - \text{Antibond } e}{2}

Heteronuclear Diatomic

Bond Order

\[ \begin{align*}
A & : 0 \\
B & : 0.5 \\
C & : 1 \\
D & : 1.5 \\
E & : 2 \\
F & : 2.5 \\
G & : 3 \\
H & : 3.5 \\
I & : 4
\end{align*} \]

Each MO looks most like the AO it is closest to.

Electron density is greatest on He

\[ \text{Back to diatomics} \]

H-F

\[ \begin{align*}
\sigma^* \\
\sigma
\end{align*} \]

2nd row diatomic

\[ \begin{align*}
2p \\
2s
\end{align*} \]

\[ \begin{align*}
\sigma^* \\
\sigma
\end{align*} \]

2nd row diatomic

\[ \begin{align*}
\sigma^* \\
\sigma
\end{align*} \]

\[ \begin{align*}
\sigma^* \\
\sigma
\end{align*} \]
Li₂
A 0  B 0.5  C 1  D 1.5  E 2  F 2.5  G 3

Unpaired electrons so it is Paramagnetic

Be₂
A 0  B 0.5  C 1  D 1.5  E 2  F 2.5  G 3

B₂
A 0  B 0.5  C 1  D 1.5  E 2  F 2.5  G 3
Is it paramagenetic (A) or diamagnetic (B)?

\[
\begin{align*}
\text{C}_2 & \quad A \quad 0 \quad B \quad .5 \quad C \quad 1 \quad D \quad 1.5 \quad E \quad 2 \quad F \quad 2.5 \quad G \quad 3 \\
\text{N}_2 & \quad A \quad 0 \quad B \quad .5 \quad C \quad 1 \quad D \quad 1.5 \quad E \quad 2 \quad F \quad 2.5 \quad G \quad 3 \\
\text{O}_2 & \quad A \quad 0 \quad B \quad .5 \quad C \quad 1 \quad D \quad 1.5 \quad E \quad 2 \quad F \quad 2.5 \quad G \quad 3
\end{align*}
\]

\[
\begin{align*}
\text{Splitting between } s \text{ and } p \text{ is greater as atomic charge increases.}
\end{align*}
\]

\[
\begin{array}{c|c|c|c|c|c|c|c|c}
\text{Atomic Orbital Energies} & 1s & 2s & 2p & 2p - 2s \\
\hline
\text{H} & -1313 & -6505 & -20204 & -29735 & -41034 & -54265 & -69268 \\
\text{Li} & -515 & -1299 & -1853 & -2482 & -3267 & -4129 & \\
\text{Be} & -814 & -1138 & -1490 & -1659 & -1917 & & \\
\text{B} & 485 & 715 & 991 & 1608 & 2212 & & \\
\text{C} & & & & & & & \\
\text{N} & & & & & & & \\
\text{O} & & & & & & & \\
\text{F} & & & & & & & \\
\end{array}
\]

The gap between 2p and 2s grows as you increase Z.