

Midterm #2 Topics

Understanding Symmetry

operation	Symbol	Element	Symbol
rotate 360°	C_n (e.g. C_2)	proper rotation axis	C_n
reflect	σ	mirror plane	σ
σ_h		horizontal	σ_h
σ_v		vertical	σ_v
σ_d		diagonal	σ_d
Invert	i	Inversion	i
rotate 360° and reflect	S_n	improper rotation axis	S_n
Identity	E	none	

Understanding Point Groups

Questions

Linear? Highly Symmetric? C_{∞} ?
 3 C_2 in right angle? C_{3v} ?
 what is the point group?

How to USE

1. Determine order
2. Determine axis
3. Determine plane
4. Determine center
5. Determine inversion
6. Determine improper rotation

- Linear: C_{∞}
- Highly Symmetric: C_{3v}
- 3 C_2 in right angle: C_{3v}
- What is the point group?

Lone pairs in Lewis structure = polar
 no lone pairs = non-polar

if there are lone pairs in the structure then the molecule is polar

- σ = bonding orbital
- σ^* = antibonding orbital
- π = bonding orbital
- π^* = antibonding orbital
- π = bonding orbital
- π^* = antibonding orbital

will be C_{3v} if no inversion center
 ex: CO

3 = gerade = symmetrical
 u = ungerade = unsymmetrical

Understanding Electron Configurations

e^- = atomic # ex: Boron!

$1s^2 2s^2 2p^1$ or $[He] 2s^2 2p^1$

$e^- = 13$

$1s^2 2s^2 2p^6 3s^2 3p^3$

$e^- = 26$

$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^6$

$[Ar] 4s^2 3d^6$

Understanding MO theory

- Two types of MOs: σ - on single bonds, π - on double and triple bonds
- Good vs. Additional
- Good: bonding molecular orbital, low energy
- Additional: antibonding molecular orbital, high energy
- Magnetic Properties
- diamagnetic: no unpaired e^-
- paramagnetic: at least 1 unpaired e^-

2 Versions of MO diagrams

Two versions of MO diagrams:

1. σ and π orbitals

2. σ and π orbitals

Center of O_2 MO diagram orbitals

- Do E config. to know which labels on MO diagram

ex: CO

$[He] 2s^2 2p^4$

$[Ar] 4s^2 3d^6$

so represents bonding

CO = $10e^-$ = $4e^-$ from C + $6e^-$ from O

$10e^-$ = $4e^-$ from C + $6e^-$ from O

$10e^-$ = $4e^-$ from C + $6e^-$ from O

$10e^-$ = $4e^-$ from C + $6e^-$ from O

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