

Resonance, Formal Charges, VSEPR

Resonance

Define –

resonance structure:

resonance hybrid:

Consider ozone, O₃:

What is the same about these two structures?

What is different?

Are these two different molecules?

Mechanism:

Combining into the resonance hybrid:

Benzene, C₆H₆ – cyclic compound with two resonance structures. Draw both resonance structures and the resonance hybrid.

Write the resonance structures for NO_3^- :

Bond order in molecules with resonance forms – partial bonding often leads to fractional bond orders:

O_3

C to C bond order in benzene

NO_3^-

Formal Charges

Define –
formal charge:

Why do we care about formal charges?

How do we calculate a formal charge?

Example: Calculate the formal charges on each O atom in each resonance form of O_3

Logic check:

Do all the formal charges add up to the charge on the molecule?

Oxygen normally has _____ bonds. What formal charge does oxygen carry when it has its usual number of bonds?

NCO⁻ - a guide to picking the more important resonance structure
3 criteria”

- 1.
- 2.
- 3.

Draw the resonance structures for NCO⁻ (hint: there are three), calculate the formal charges, determine the most important one.

Why did you choose the structure you did?

Exceptions to the octet rule

Define –
electron deficient:

free radical:

expanded valence shell:

1. Two examples of e⁻ deficiency –

Using formal charges, explain why a full octet for Be and B would be unlikely.

So, how does a deficient atom attain an octet?

2. An example of a free radical

The lone electron in a free radical causes them to have two important properties:

- 1.
- 2.

Where on the periodic table do most odd electron molecules find their central atom?

Show the two resonance forms of NO_2 and calculate formal charges for each atom in each form.

Reactivity of radicals along with the formal charges helps determine which is more important:

3. Expanded valence shells – a few examples

Sulfur:

SF_6

H_2SO_4 (two resonance structures)

Phosphorus:

PCl_3

PCl_5

Draw the Lewis structures for H_3PO_4 and choose the most likely structure.

Draw the Lewis structure for BFCl_2

VSEPR – Giving 3D shape to molecules

Define –

VSEPR:

molecular shape:

bond angle:

The shapes, how to categorize them, and some examples

Note –

A stands for the central atom

X stands for other atoms

E stands for lone pairs

Two electron groups – Linear arrangement (one class)

Class:

Shape:

Bond angle:

Examples:

Three electron groups – Trigonal planar arrangement (two classes)

Class:

Shape:

Bond angle:

Number of bonding groups:

Examples:

Class:

Shape:

Bond angle:

Number of bonding groups:

Examples:

Four electron groups – Tetrahedral arrangement (three classes)

Class:

Shape:

Bond angle:

Number of bonding groups:

Examples:

Class:

Shape:

Bond angle:

Number of bonding groups:

Examples:

Class:

Shape:

Bond angle:

Number of bonding groups:

Examples:

Five electron groups – Trigonal bipyramidal arrangement (four classes)

Class:

Shape:

Bond angle:

Number of bonding groups:

Examples:

Class:

Shape:

Bond angle:

Number of bonding groups:

Examples:

Class:

Shape:

Bond angle:

Number of bonding groups:

Examples:

Class:

Shape:

Bond angle:

Number of bonding groups:

Examples:

Six electron groups – Octahedral arrangement (three classes)

Class:

Shape:

Bond angle:

Number of bonding groups:

Examples:

Class:

Shape:

Bond angle:

Number of bonding groups:

Examples:

Class:

Shape:

Bond angle:

Number of bonding groups:

Examples:

Steps to using VSEPR theory to determine molecular shape:

1.

2.

3.

4.

Place the following into the above categories:

PF₃, COCl₂, SbF₅, ClF₅, CS₂, PbCl₂, CBr₄, SF₂, ClF₃, ICl₂⁻, SOF₄