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[TP] Which molecule is more polar? ($\chi_{\text{H}} = 2.1$, $\chi_{\text{B}} = 2.04$, $\chi_{\text{N}} = 3.04$, $\chi_{\text{F}} = 3.98$)

27% 1. NH_3 (trigonal pyramid)
 58% 2. BF_3 (trigonal planar)
 15% 3. Polarity is the same

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 Tuesday, October 15, 2019

- Resonance hybrids
- Exceptions to octet rule
- Electronegativity and bond character
- Bond polarity
- Molecular geometry

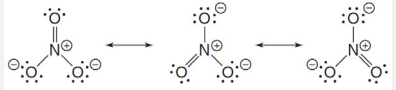
Next: Molecular polarity; Begin ch9: Covalent bonding

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
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Lewis formula of NO_3^- (nitrate)

Alternative equivalent formulas are known as resonance forms.



Bonding is an equal mixture of each resonance form, known as a resonance hybrid.



The shared electrons are said to be delocalized across the four atoms, represented as a resonance hybrid. The mixture does not vary with time.

Each bond is 1/3 of the way between single and double.

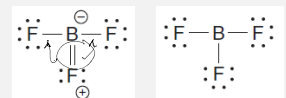
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Exceptions to the octet "rule"

Octet deficient: BF_3



Single bonds more stable, based on formal charge.

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Exceptions to the octet "rule"

Odd number of electrons: NO_2 7

$\frac{1}{2} \text{N} - \frac{1}{2} \text{O}$

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Exceptions to the octet "rule"

Expanded octet (period 3 onward): POCl_3

$5 + 6 + 21 = 32 e^-$
 16 pairs

Expanded octet more stable, based on formal charge.

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Electronegativity

Formal charge assumes electrons between atoms are shared equally.

Unless two connected atoms are identical, sharing always favors one atom.

Electronegativity is a relative measure the tendency of an atom to attract electrons shared with another atom in a covalent bond.

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Electronegativity, χ (Greek letter chi, "hee")

Electronegativity is a relative measure the tendency of an atom to attract electrons shared with another atom in a covalent bond.

1 H 2.1	2 He —																
3 Li 0.98	4 Be 1.57	5 B 2.04	6 C 2.55	7 N 3.04	8 O 3.44	9 F 3.98	10 Ne —										
11 Na 0.93	12 Mg 1.31	13 Al 1.61	14 Si 1.90	15 P 2.19	16 S 2.58	17 Cl 3.16	18 Ar —										
19 K 0.82	20 Ca 1.09	21 Sc 1.36	22 Ti 1.54	23 V 1.63	24 Cr 1.66	25 Mn 1.55	26 Fe 1.83	27 Co 1.88	28 Ni 1.91	29 Cu 1.90	30 Zn 1.65	31 Ga 1.81	32 Ge 2.01	33 As 2.18	34 Se 2.35	35 Br 2.96	36 Kr —
37 Rb 0.82	38 Sr 0.95	39 Y 1.22	40 Zr 1.33	41 Nb 1.6	42 Mo 2.16	43 Tc 1.9	44 Ru 2.2	45 Rh 2.28	46 Pd 2.29	47 Ag 1.93	48 Cd 1.69	49 In 1.78	50 Sn 1.96	51 Sb 2.05	52 Te 2.1	53 I 2.46	54 Xe —
55 Cs 0.79	56 Ba 0.89	57-71 HF 1.1-1.2	72 Hf 1.3	73 Ta 1.5	74 W 2.36	75 Re 1.9	76 Os 2.2	77 Ir 2.29	78 Pt 2.28	79 Au 2.54	80 Hg 2.01	81 Tl 2.04	82 Pb 2.33	83 Bi 2.02	84 Po 2.0	85 At 2.2	86 Rn —

F > O > Cl > N > S > C > P > H
3.98 3.44 3.16 3.04 2.58 2.55 2.19 2.1

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Electronegativity, χ (Greek letter chi, "hee")

Electronegativity is a relative measure the tendency of an atom to **attract electrons** shared with another atom in a covalent bond.

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Bond polarity

The greater the **electronegativity difference** of two covalently bonded atoms, the **more unequal the sharing** of the electrons forming the covalent bond.

Bond character:	Covalent	Polar covalent	Ionic
Electronegativity difference:	$\approx 0 - 0.3$	$\approx 0.4 - 2.0$	$\approx 2.1 - 4.0$

BrI: $2.96 - 2.66 = 0.30$, **covalent**

HCl: $3.16 - 2.1 = 1.0$, **polar covalent**

NaCl: $3.16 - 0.93 = 2.23$, **ionic**

Please keep in mind that these definitions are qualitative, since sharing is **always unequal unless the bonded atoms are identical**.

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[TP] Which bond is **more polar**? ($\chi_{\text{H}} = 2.1$, $\chi_{\text{B}} = 2.04$, $\chi_{\text{N}} = 3.04$, $\chi_{\text{F}} = 3.98$)

14% 1. N-H

80% 2. B-F

2% 3. Polarity is the same

Handwritten calculations:

$$\begin{array}{r} 3.98 \\ - 2.04 \\ \hline 1.94 \end{array}$$

$$\begin{array}{r} 3.04 \\ - 2.1 \\ \hline 0.94 \end{array}$$

Handwritten Lewis structure:

$$\begin{array}{c} \text{F} - \text{B} - \text{F} \\ | \\ \text{F} \end{array}$$

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Predicting molecular geometries

How atoms are **arranged in three dimensions** around their **central atom** is determined by the **steric number (SN)** the central atom.

SN = attached atoms + lone pairs

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SN = attached atoms + lone pairs

What is SN of C in CO_2 ?
 $4 + 12 = 16 \text{ e}^-$ or 8 pairs
 SN = 2: **Two** attached atoms and **zero** lone pairs

What is the SN of O in H_2O ?
 $2 + 6 = 8 \text{ e}^-$
 SN = 4: **Two** attached atoms and **two** lone pairs

What is the SN of N in NO_2^- ?
 $5 + 6 + 1 = 12 \text{ e}^-$
 SN = 3: **Two** attached atoms and **one** lone pair

Handwritten Lewis structures: $\text{O}=\text{C}=\text{O}$, $\text{H}-\text{O}-\text{H}$, and $\text{O}=\text{N}-\text{O}$ with a negative charge on the nitrogen atom.

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SN = attached atoms + lone pairs

What is the SN of B in BF_3 ?
 SN = 3: **Three** attached atoms and **zero** lone pairs

What is SN of S in SF_4 ?
 SN = 5: **Four** attached atoms and **one** lone pair

What is the SN of S in SF_6 ?
 SN = 6: **Six** attached atoms and **zero** lone pairs

Handwritten Lewis structure for SF_6 showing six fluorine atoms around a central sulfur atom.

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Predicting molecular geometries: SN = 2

What is SN of C in CO_2 ?
 SN = 2: **Two** attached atoms and **zero** lone pairs

Diagram showing a central atom (white) bonded to two atoms (red) in a straight line within a circle. Labeled AX_2 linear.

Shape is **linear**, bond angle is **180°**

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Predicting molecular geometries: SN = 3

What is the SN of N in NO_2^- ?
 SN = 3: **Two** attached atoms and **one** lone pair

Two diagrams: one for AX_3 trigonal planar (three red atoms around a white central atom) and one for AX_2E bent (two red atoms and one green lone pair around a white central atom).

Shape is **bent**, bond angle **a bit less than 120°**

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Predicting molecular geometries: SN = 4

What is the SN of O in H_2O ?

SN = 4: **Two** attached atoms and **two** lone pairs

AX_4 tetrahedral
 AX_3E trigonal pyramidal
 AX_2E_2 bent

Shape is **bent**, bond angle a **little less than 109.5°**

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Predicting molecular geometries: SN = 5

What is SN of S in SF_4 ?

SN = 5: **Four** attached atoms and **one** lone pair

AX_5 trigonal bipyramidal
 AX_4E seesaw-shaped
 AX_3E_2 T-shaped
 AX_2E_3 linear

Shape is **seesaw**, bond angles are a **little less than 180° , 120° , and 90°**

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Predicting molecular geometries: SN = 6

What is the SN of S in SF_6 ?

SN = 6: **Six** attached atoms and **zero** lone pairs

AX_6 octahedral
 AX_5E square pyramidal
 AX_4E_2 square planar

Shape is **octahedral**, bond angles are **90°**

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