

Lecture 16 CH101 A1 (MWF 9:05 am) Fall 2019 Copyright © 2019 Dan Dill dan@bu.edu

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

41% 1. NH_3 (trigonal pyramid)
 55% 2. BF_3 (trigonal planar)
 4% 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
- Molecular polarity

Next: Molecular polarity; Begin ch9: Covalent bonding

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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

$\frac{1}{2}$ N $\frac{1}{2}$

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Exceptions to the octet "rule"

Expanded octet (period 3 onward): POCl_3

$32 e^- = 16 \text{ pairs}$

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																	2	
H 1.0																	He —	
3	4											5	6	7	8	9	10	
Li 0.98	Be 1.57											B 2.04	C 2.55	N 3.04	O 3.44	F 3.98	Ne —	
11	12											13	14	15	16	17	18	
Na 0.93	Mg 1.31											Al 1.61	Si 1.90	P 2.19	S 2.58	Cl 3.16	Ar —	
19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	
K 0.82	Ca 1.00	Sc 1.36	Ti 1.54	V 1.63	Cr 1.66	Mn 1.55	Fe 1.83	Co 1.88	Ni 1.91	Cu 1.90	Zn 1.65	Ga 1.81	Ge 2.01	As 2.18	Se 2.35	Br 2.96	Kr —	
37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	
Rb 0.82	Sr 0.95	Y 1.22	Zr 1.33	Nb 1.6	Mo 2.16	Tc 1.9	Ru 2.2	Rh 2.28	Pd 2.20	Ag 1.93	Cd 1.69	In 1.78	Sn 1.96	Sb 2.05	Te 2.1	I 2.66	Xe —	
55	56	57-71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	
Cs 0.79	Ba 0.89	1.1-1.2		Hf 1.3	Ta 1.5	W 2.36	Re 1.9	Os 2.2	Ir 2.20	Pt 2.28	Au 2.54	Hg 2.00	Tl 2.04	Pb 2.33	Bi 2.02	Po 2.0	At 2.2	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.

The graph shows Pauling electronegativity on the y-axis (0 to 4.0) and atomic number on the x-axis (0 to 100). Key points are labeled: Li, Na, K, Rb, Cs, F, Cl, Br, I, At, and Fr. The diagram shows electronegativity increasing from left to right and bottom to top, with the highest values in the top right and lowest in the bottom left.

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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			

Handwritten notes: "most equal" for BrI, "most unequal" for NaCl.

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**? ($\chi_H = 2.1$, $\chi_B = 2.04$, $\chi_N = 3.04$, $\chi_F = 3.98$)

- 9% 1. N-H
- 86% **2. B-F**
- 4% 3. Polarity is the same

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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.

$SN = \text{attached atoms} + \text{lone pairs}$

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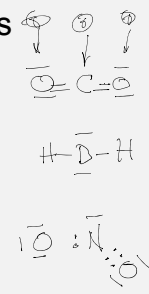
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SN = attached atoms + lone pairs

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

What is the SN of O in H_2O ?
 SN = 4: **Two** attached atoms and **two** lone pairs

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



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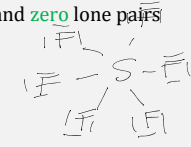
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SN = attached atoms + lone pairs

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



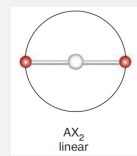
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Predicting molecular geometries: SN = 2

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



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

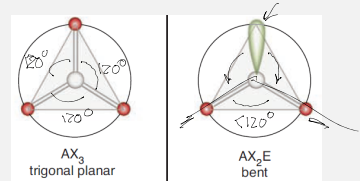
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Predicting molecular geometries: SN = 3

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



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 H₂O?

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

AX₄ tetrahedral AX₃E trigonal pyramidal AX₂E₂ 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 SF₄?

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

AX₅ trigonal bipyramidal AX₄E seesaw-shaped AX₃E₂ T-shaped AX₂E₃ 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 SF₆?

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

AX₆ octahedral AX₅E square pyramidal AX₄E₂ square planar

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

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[TP] What is the molecular shape of ClF₃?

- 0% 1. Linear
- 4% 2. Trigonal planar
- 15% 3. Tetrahedral
- 26% 4. Trigonal pyramidal
- 11% 5. Bent
- 15% 6. Seesaw
- 29% 7. T-shaped
- 1% 8. None of these

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Predicting molecular geometries: SN = 5

What is SN of Cl in ClF_3 ?

SN = 5: **Three** attached atoms and **two** lone pairs

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

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

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Predicting molecular geometries: SN = 5

What is SN of Cl in ClF_3 ?

SN = 5: **Three** attached atoms and **two** lone pairs

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

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