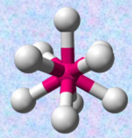
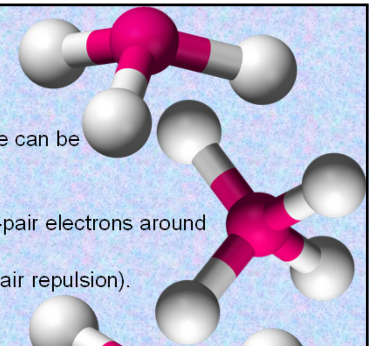
Shape of molecules



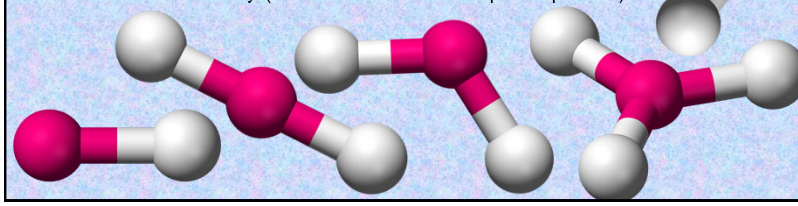
8

Shapes of Molecules



The *three-dimensional shape* of a molecule can be predicted by

- the number of bonding groups and lone-pair electrons around the central atom
- VSEPR theory (valence-shell-electron-pair repulsion).

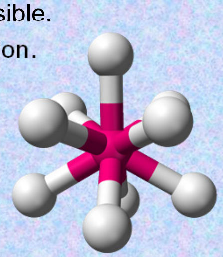


9

Valence-Shell Electron-Pair Repulsion Theory (VSEPR)

In the **valence-shell electron-pair repulsion (VSEPR) theory**, the electron groups around a central atom

- are arranged as far apart from each other as possible.
- have the least amount of electron-electron repulsion.
- are used to predict the molecular shape.

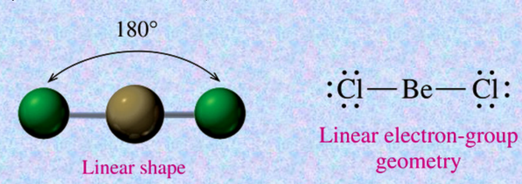


10

Two Electron Groups

In a molecule of $BeCl_2$,

- there are two electron groups bonded to the central atom, Be (Be is an exception to the octet rule).



- to minimize repulsion, the arrangement of two electron groups is 180°, or opposite each other.
- the shape of the molecule is **linear.**

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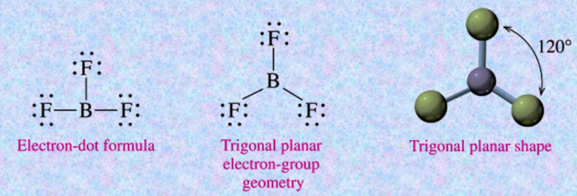
11

11

Three Electron Groups

In a molecule of BF_3,

- three electron groups are bonded to the central atom B (B is an exception to the octet rule).

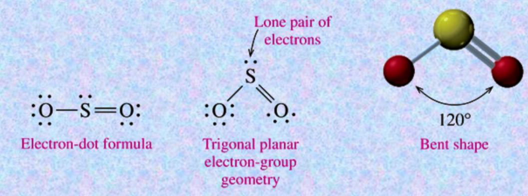


- repulsion is minimized with 3 electron groups at angles of 120°.
- the shape is **trigonal planar.**

Three Electron Groups with a Lone Pair

In a molecule of SO_2,

- S has 3 electron groups; 2 electron groups bonded to O atoms and one lone pair.

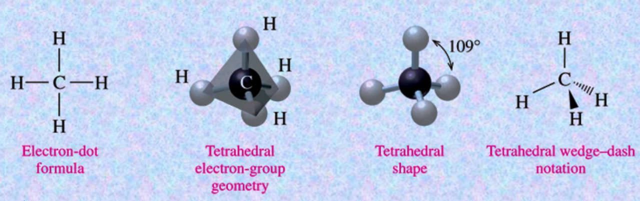


- repulsion is minimized with the electron groups at angles of 120°, a trigonal planar arrangement.
- the shape is determined by the two O atoms bonded to S, giving SO_2 a **bent (~120°)** shape.

Four Electron Groups

In a molecule of CH_4,

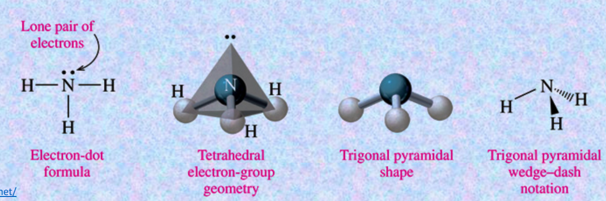
- there are four electron groups around C.
- repulsion is minimized by placing four electron groups at angles of 109°, which is a **tetrahedral** arrangement.
- the four bonded atoms form a **tetrahedral** shape.



Four Electron Groups with a Lone Pair

In a molecule of NH_3,

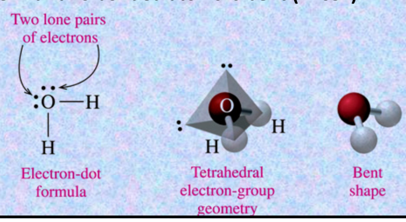
- three electron groups bond to H atoms, and the fourth one is a lone (nonbonding) pair.
- repulsion is minimized with 4 electron groups in a **tetrahedral** arrangement.
- the three bonded atoms form a **pyramidal (~109°)** shape.



Four Electron Groups with Two Lone Pairs

In a molecule of H_2O,

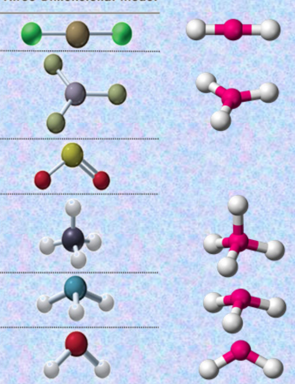
- two electron groups are bonded to H atoms and two are lone pairs (4 electron groups).
- four electron groups minimize repulsion in a **tetrahedral** arrangement.
- the shape with two bonded atoms is **bent (~109°).**



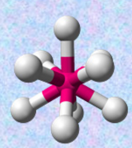
16

Molecular Shapes for Bonded Atoms

Electron Groups	Electron-Group Arrangement	Bonded Atoms	Lone Pairs	Bond Angle	Molecular Shape	Example	Three-Dimensional Model
2	**Linear**	2	0	180°	Linear	$BeCl_2$	
3	**Trigonal planar**	3	0	120°	Trigonal planar	BF_3	
		2	1	120°	Bent	SO_2	
4	**Tetrahedral**	4	0	109°	Tetrahedral	CH_4	
		3	1	109°	Trigonal pyramidal	NH_3	
		2	2	109°	Bent	H_2O	



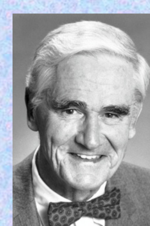
17



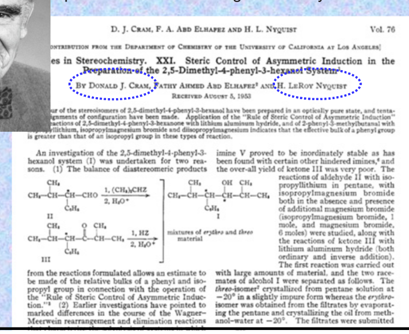
Lewis Structures

18

'My' process for Lewis Structures



Donald James Cram was an American chemist who shared the 1987 Nobel Prize in Chemistry with Jean-Marie Lehn and Charles J. Pedersen "for their development and use of molecules with structure-specific interactions of high selectivity."



D. J. Cram, F. A. Abd Elhafez and H. L. Nyquist Vol. 76

[Contribution from the Department of Chemistry of the University of California at Los Angeles]

...es in Stereochemistry. XXI. Steric Control of Asymmetric Induction in the Preparation of the 2,5-Dimethyl-4-phenyl-3-hexanol System

By Donald J. Cram, Fathy Ahmed Abd Elhafez and H. LeRoy Nyquist

Received August 5, 1953

...ur of the stereoisomers of 2,5-dimethyl-4-phenyl-3-hexanol have been prepared in an optically pure state, and tenta... ...gnments of configuration have been made. Application of the "Rule of Steric Control of Asymmetric Induction" ...actions of 2,5-dimethyl-4-phenyl-3-hexanone with lithium aluminum hydride, and of 2-phenyl-3-methylbutanal with ...yllithium, isopropylmagnesium bromide and diisopropylmagnesium indicates that the effective bulk of a phenyl group is greater than that of an isopropyl group in these types of reaction.

An investigation of the 2,5-dimethyl-4-phenyl-3-hexanol system (I) was undertaken for two reasons. (1) The balance of diastereomeric products ...

imine V proved to be inordinately stable as has been found with certain other hindered imines,[4] and the over-all yield of ketone III was very poor. The reactions of aldehyde II with isopropyllithium in pentane, with isopropylmagnesium bromide both in the absence and presence of additional magnesium bromide ...

H. LeRoy Nyquist, Professor of Organic Chemistry at California State University, Northridge – b.8/12/1929 – d.7/20/2014.

My mentor and friend.

He is the one that over five years of research instilled in my the following method.

19

Drawing Electron-Dot Formulas

Arrange atoms

Determine the number of valence electrons

Place valence electrons on each atom

Make sure all atoms have a complete shell

Try rearranging atoms or double bonds

20

Gilbert Lewis

The subject of chemical bonding is at the heart of chemistry. In 1916 Gilbert Newton Lewis (1875–1946) published his seminal paper suggesting that a chemical bond is a pair of electrons shared by two atoms.

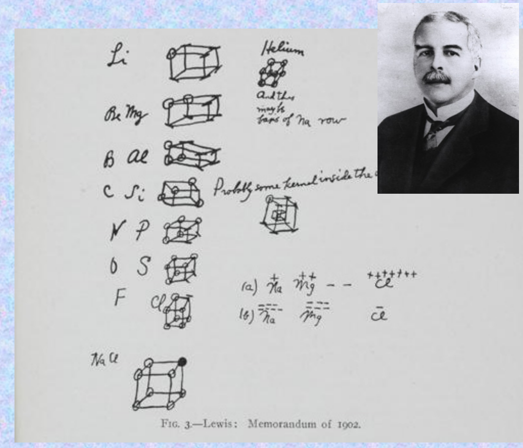
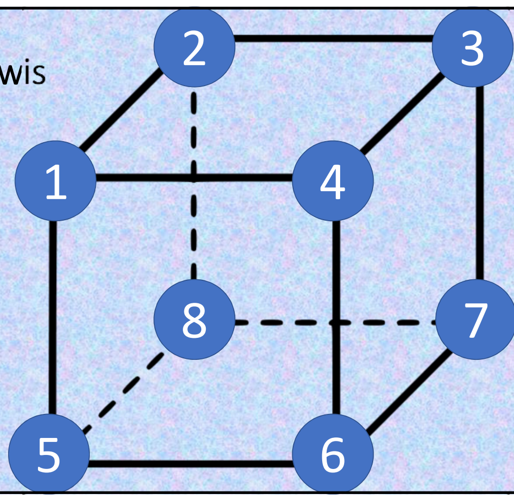


Fig. 3—Lewis: Memorandum of 1902.

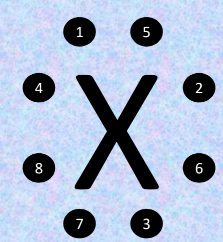
21

Gilbert Lewis

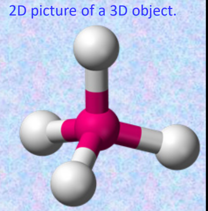


22

Drawing the valence electrons



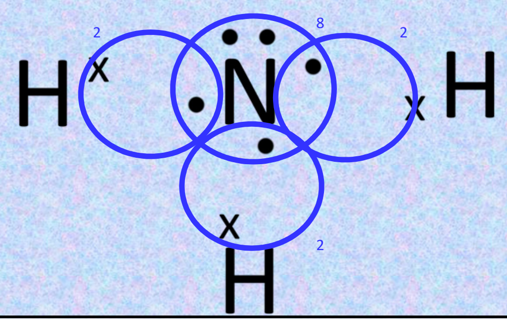
Remember that this is a 2D picture of a 3D object.



23

Draw the Electron-Dot Formula for NH_3

Arrange the atoms, place the valence electrons



24

Exceptions to the Octet Rule

Not all atoms have octets.

- Some can have less than an octet, such as
  - H, which requires only 2 electrons,
  - B, which requires only 6 electrons, and
  - Be, which requires only 4 electrons.
- Some can have expanded octets, such as
  - P, which can have 10 electrons,
  - S, which can have 12 electrons, and
  - Cl, Br and I, which can have 14 electrons

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25

25

Single and Multiple Bonds

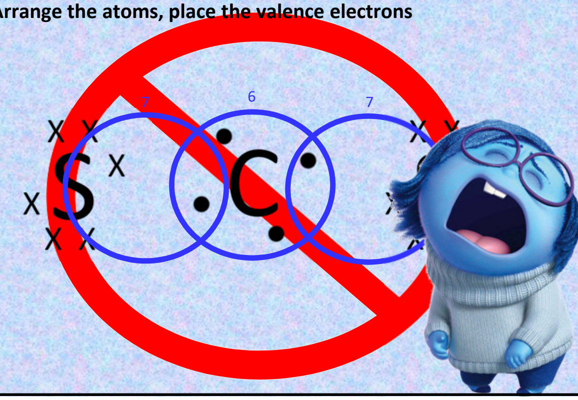
In many covalent compounds, atoms share two or three pairs of electrons to complete their octets.

- In a **single bond**, one pair of electrons is shared.
- In a **double bond**, two pairs of electrons are shared.
- In a **triple bond**, three pairs of electrons are shared.

26

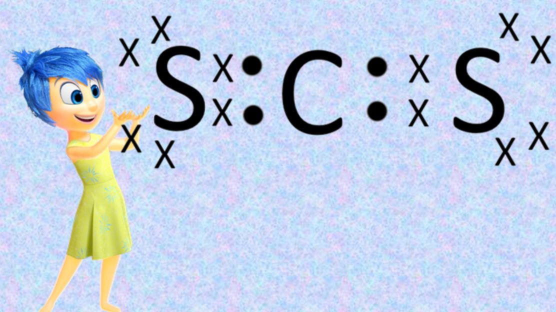
Draw the Electron-Dot Formula for CS_2

Arrange the atoms, place the valence electrons



27

Draw the Electron-Dot Formula for CS_2



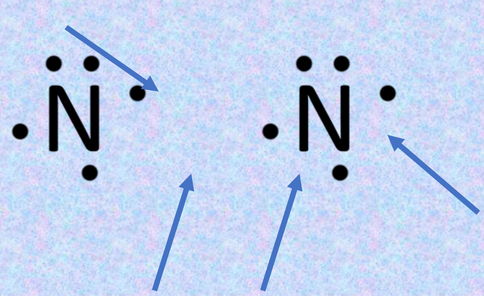
28

Try Nitrogen Gas

$$N_2$$

29

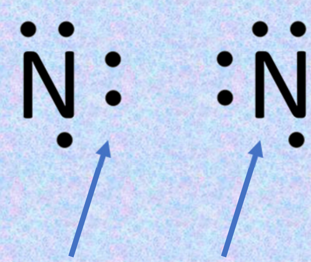
Try Nitrogen Gas – Single Bond



4-Lone Electrons ☹

30

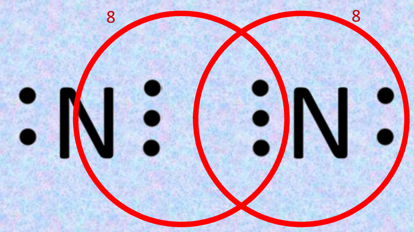
Try Nitrogen Gas – Double Bond



2-Lone Electrons ☹

31

Try Nitrogen Gas – Triple Bond



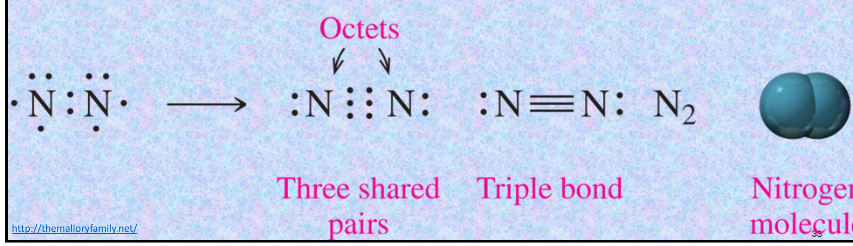
0-Lone Electrons ☺

32

A Nitrogen Molecule has a Triple Bond

In a nitrogen molecule, N_2,

- each N atom shares 3 electrons,
- each N atom attains an octet, and
- the sharing of 3 sets of electrons is called a triple bond.



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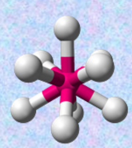
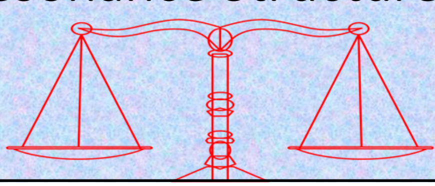
33

Resonance Structures





34

Resonance Structures

Resonance structures are

- two or more electron-dot formulas for the same arrangement of atoms.
- related by a double-headed arrow (↔).
- written by changing the location of a double bond between the central atom and a different attached atom.

35

Writing Resonance Structures for SO_2

Sulfur dioxide has two resonance structures.

Step 1 **Determine the arrangement of atoms.** In SO_2, the S atom is the central atom.

O S O

Step 2 **Determine the total number of valence electrons.**

Element	Group	Atoms	Valence Electrons	Total
S	6A (16)	1 S	1 x 6 *e*−	6 *e*−
O	6A (16)	2 O	2 x 6 *e*−	12 *e*−

SO_2 = 18 *e*−

This is the book's method

36

Writing Resonance Structures for SO_2

Step 3 **Attach each bonded atom to the central atom with a pair of electrons.**

O : S : O or O—S—O

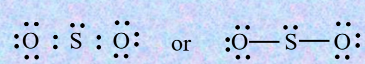
This is the book's method

37

Writing Resonance Structures for SO_2

Step 4 **Place the remaining electrons using single or multiple bonds to complete the octets.**

The remaining 14 electrons are drawn as lone pairs of electrons to complete the octets of the O atoms, but not the S atom.



This is the book's method

38

Writing Resonance Structures for SO_2

Step 4 **Continued:** To complete the octet for S, an additional lone pair from one of the O atoms is shared to form a double bond.

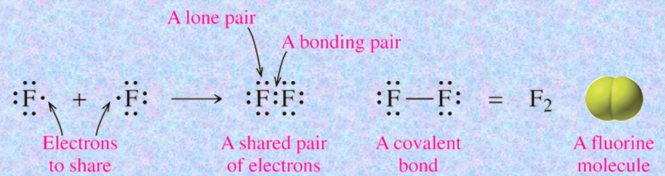
Because the shared lone pair of electrons can come from either O atom, two resonance structures can be drawn.

This is the book's method

39

Electron-Dot Formulas of Covalent Molecules

In a fluorine (F_2) molecule, the F atoms
- share one of their valence electrons.
- acquire an octet.
- form a covalent bond.



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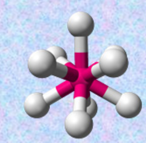
40

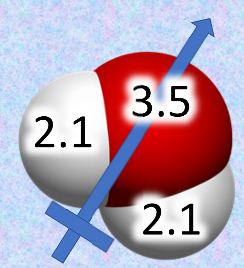
40

Electronegivity



41

Electronegivity of a Molecule



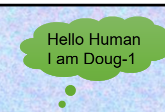
Electronegativity Increases →

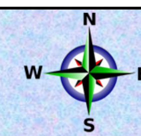
Electronegativity Decreases ↓

H 2.1

1 Group 1A	2 Group 2A	13 Group 3A	14 Group 4A	15 Group 5A	16 Group 6A	17 Group 7A	18 Group 8A
Li 1.0	Be 1.5	B 2.0	C 2.5	N 3.0	O 3.5	F 4.0	
Na 0.9	Mg 1.2	Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0	
K 0.8	Ca 1.0	Ga 1.6	Ge 1.8	As 2.0	Se 2.4	Br 2.8	
Rb 0.8	Sr 1.0	In 1.7	Sn 1.8	Sb 1.9	Te 2.1	I 2.5	
Cs 0.7	Ba 0.9	Tl 1.8	Pb 1.9	Bi 1.9	Po 2.0	At 2.1	

42





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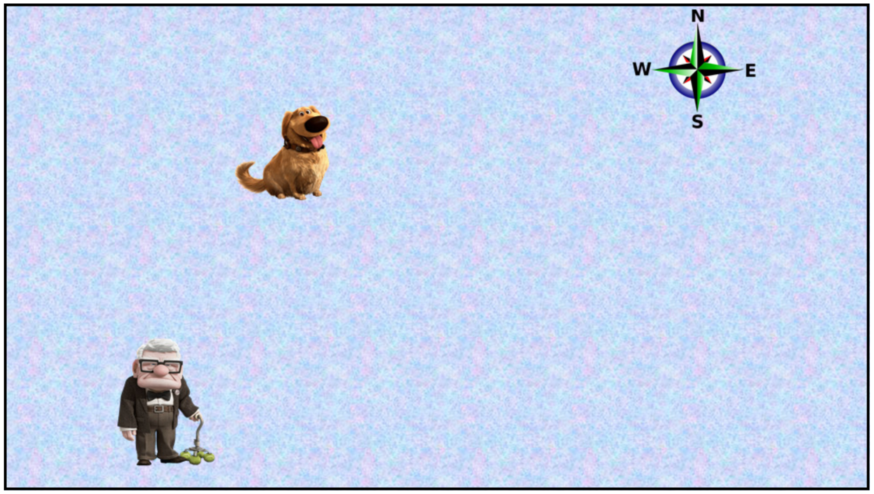

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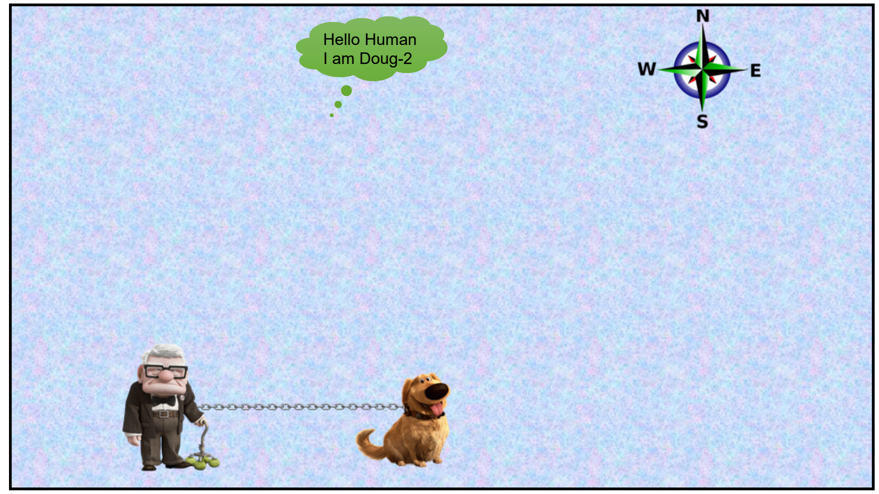

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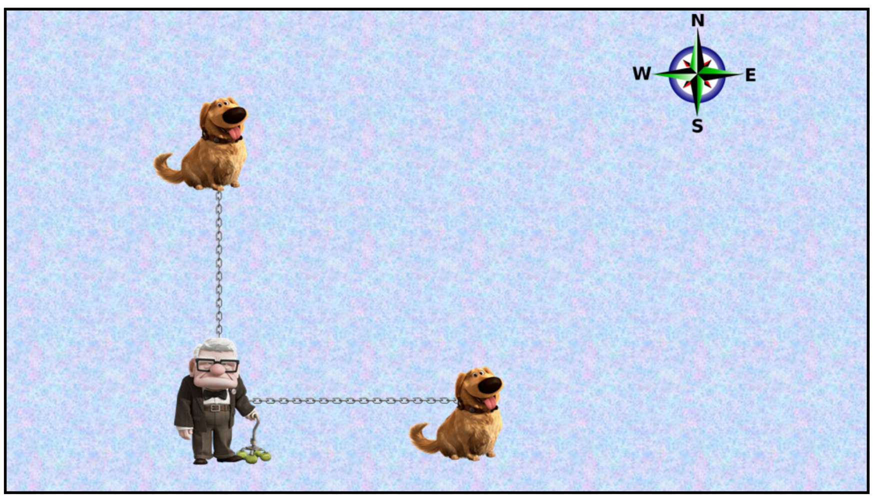

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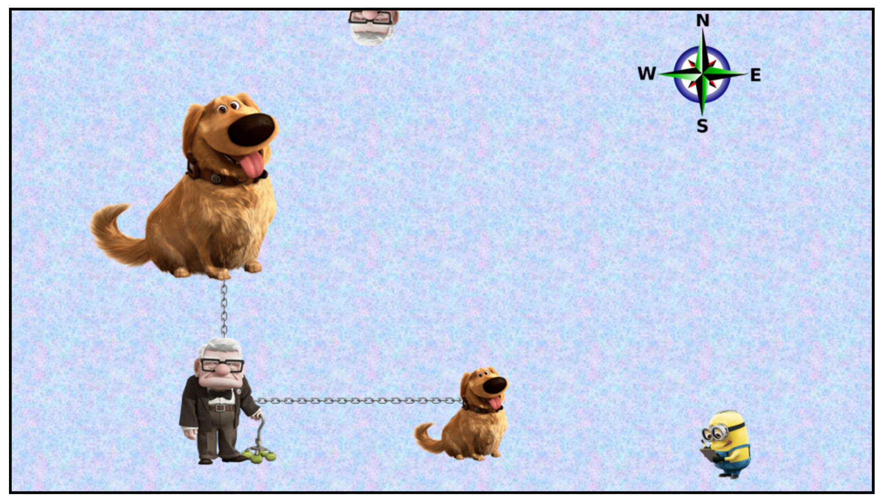
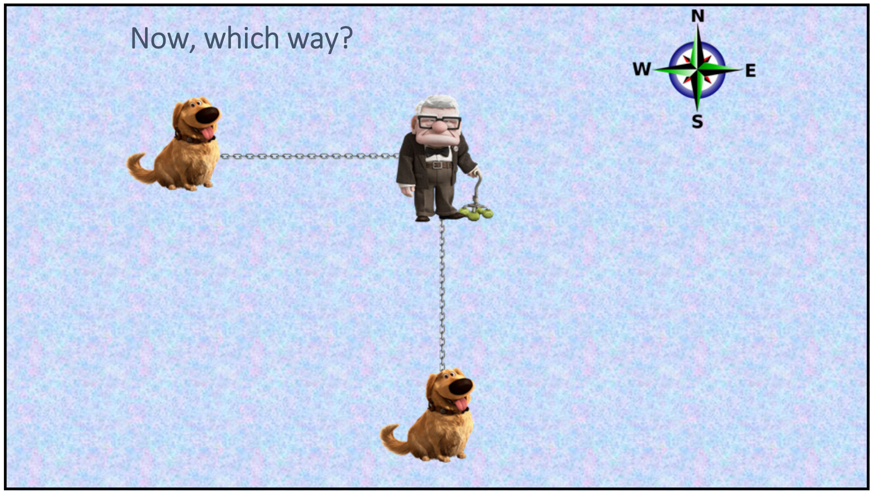
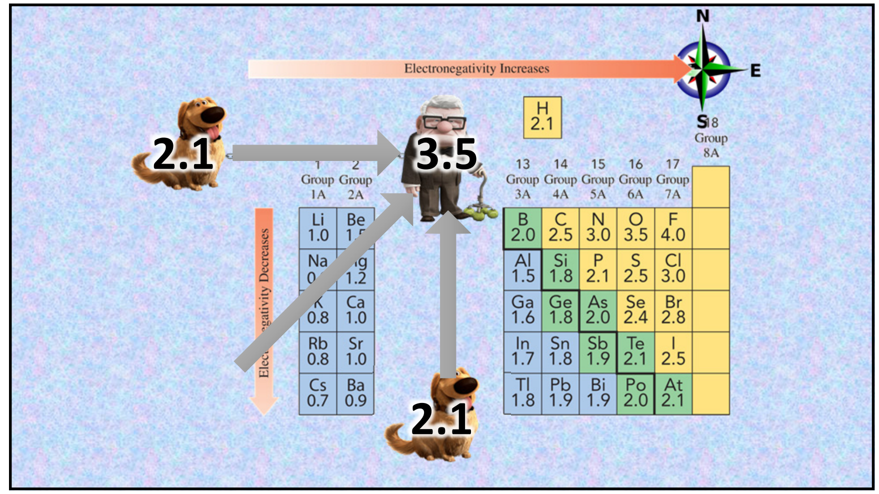


47


Now, which way?
N
W
E
S

48


Electronegativity Increases
N
E
S
2.1
3.5
2.1
H 2.1
1 Group 1A
2 Group 2A
13 Group 3A
14 Group 4A
15 Group 5A
16 Group 6A
17 Group 7A
18 Group 8A
Li 1.0
Ca 1.0
Rb 0.8
Sr 1.0
Cs 0.7
Ba 0.9
B 2.0
C 2.5
N 3.0
O 3.5
F 4.0
Al 1.5
Si 1.8
P 2.1
S 2.5
Cl 3.0
Ga 1.6
Ge 1.8
As 2.0
Se 2.4
Br 2.8
In 1.7
Sn 1.8
Sb 1.9
Te 2.1
I 2.5
Tl 1.8
Pb 1.9
Bi 1.9
Po 2.0
At 2.1

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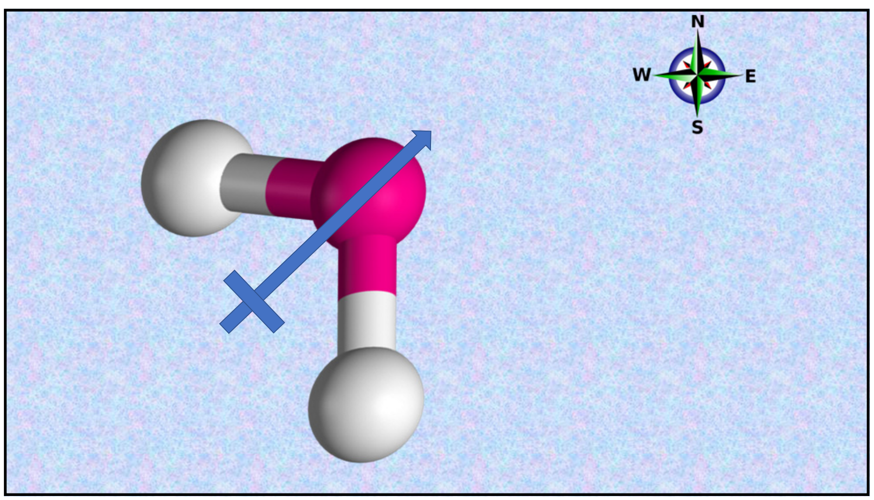
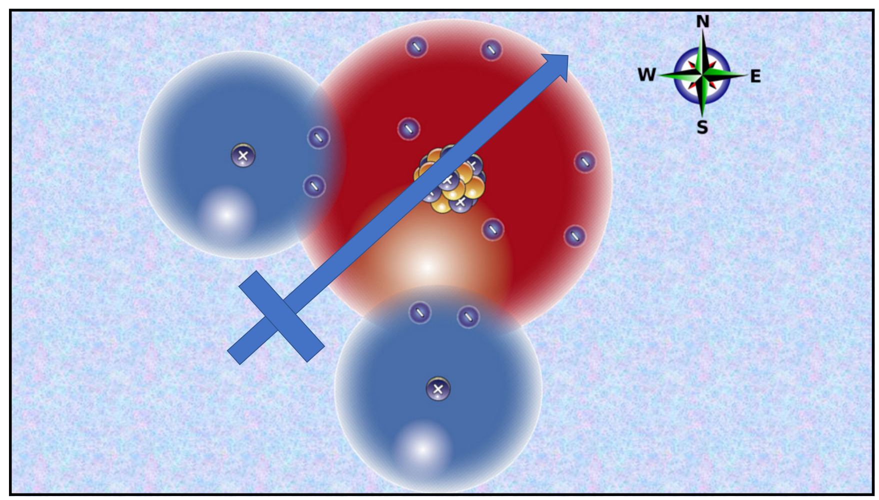
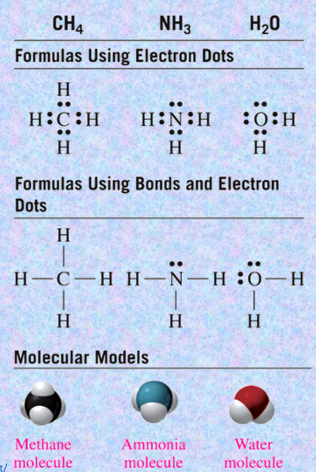

N
W
E
S

50


N
W
E
S

51

Electron-Dot Formulas for Some Covalent Compounds



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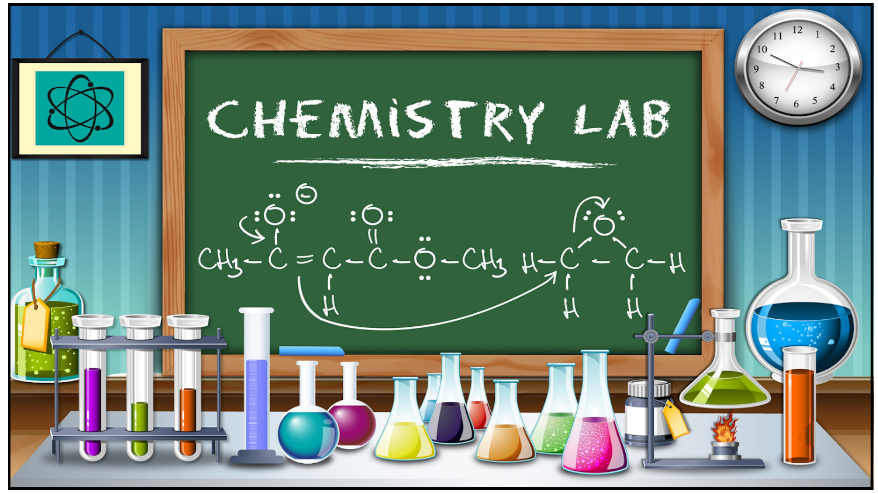
52

52



53