

CH301 Worksheet 6: Creating 3 dimensional structures of molecules to determine polarity

A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U
Name molecular formula	Initial layout EN values	Ionic or Covalent bond	N	A	S	B	Octet rule?	Double or triple	Resonance?	Lewis dot structure	#e- rich regions	Electronic geometry	Hybridization	Bond angle	Bonding pairs	Unbonded pairs	Molecular geometry	VSEPR structure	VSEPR with dipoles	Polar?
H <sub>2</sub> O	3.5 1.0 2.4	C	12	8	4	2	Y	N	N		4	tetrahedral	sp <sup>3</sup>	105.5	2	2	bent			Y
NH <sub>3</sub>	H 1.0 N 3.0 H 2.1	C	14	8	6	3	Y	N	N		4	tetrahedral	sp <sup>3</sup>	109.5	3	1	trigonal pyramidal			Y
I <sub>3</sub>	I 0 I 0 I 0	C	24	22	2	2	N	N	N		5	trigonal bipyramidal	sp <sup>3</sup> d	120 90 180	2	3	linear			N
SO <sub>2</sub>	0.35 5.3 0	C	24	18	6	2	Y	N	Y		3	trigonal bipyramidal	sp <sup>2</sup>	120	2	1	bent			Y

Explanation of columns:

- B Create symmetrical layout of atoms and assign EN values to each atom
- D Calculate  $\Delta EN > 1.5$ , bond is ionic. If  $\Delta EN < 1.5$ , bond is covalent.
- D-G Assign needed (N), available (A), shared electrons (S) and bond sites (B) for Lewis dot determination
- H Does structure follow octet rule. If yes, then answer J and K as below.
- I Double or triple bonds in molecule is S/2/B is integer > 1
- J Resonance if (S/2)/B is not an integer
- K Create Lewis dot structure
- L Count regions of electron density to perform VSEPR and VB determinations
- M-O Electronic geometry, hybridization bond angle from regions of electron density
- P-R Bonding and nonbonding electron pairs around central atom and molecular geometry that results.
- S Draw VSEPR 3-D structure including all available electrons (column E)
- T,U Draw VSEPR 3-D structure with dipole moments ( $\Delta EN$ ) from column B. If  $\Sigma \Delta EN = 0$ , then non-polar,  $\Sigma \Delta EN \neq 0$  then polar.