VSEPR Valent Shell Electron Pair Repulsion method of Covalent Bond formation

First Name: _____ Surname: _____ Group N° _____ dep Med Bio Chem

Task for student practical introduction for the use of Interactive Molecule viewers:

RasWin ChemScape MDLi MAGE4 FireFox3.5.5 ISIS

Task choose the Homepage: http://aris.gusc.lv/06Daugavpils/Research/VSEPR-A.doc

1. On HTML browser address:
http://aris.gusc.lv/ChemFiles/ComplexCompounds/PensilvaniaLebanonUniv/PensilvaniaLebanonUniv/VSEPR_table_C0.html
lunch using bookmarks of the Folder "BioChem" The **VSEPR** for studies of simple molecules
You have under investigation them:

at Display conditions: (on Menu Stripe or pressing 2nd button of mouse)

Stick
Ball & Stick
Spacefill

2. To explore the given molecules in HTLM home page identify simple-single sigma **σ** bond as first and add the secondary real present pi **π** bond in double and triple bonding features.

2. To investigate the atoms making up the molecule structure using CPK **Corey**, **Pauling**, **Koltun** publication in 1965 **Nature** & **USA Patent** for atomic modeling CPK atoms color scheme

at Display conditions: **Stick** **Ball & Stick** **Spacefill**

Atom Name	Symbol	Color	Valence Number
Carbon	C	**Gray** lightly or **Black**	**4**
Hydrogen	H	White	**1**
Oxygen	O	**Red**	**2** (donor acceptor ligand up to 4)
Nitrogen	N	**Bluish**	**3** +1(donor acceptor ligand up to 4)
Sulfur	S	**Yellow**	**-2** , **+6**
Phosphor	P	**Yellow** Intensive dark	**5** (& 3)
Sodium ion	Na^+	**Blue**	**+1** (coordination up to 6)
Magnesium ion	Mg^{2+}	**Green**	**+2** (coordination up to 6)
Calcium ion	Ca^{2+}	**Gray** Dark	**+2** (coordination up to 6)
Aluminium ion	Al^{3+}	**Gray** Dark	**+3** (coordination up to 6)
Iron ion	Fe^{2+}	**Yellow** Gray	**+2** (coordination up to 6)
Iron ion	Fe^{3+}	**Yellow** Gray	**+3** (coordination up to 6)

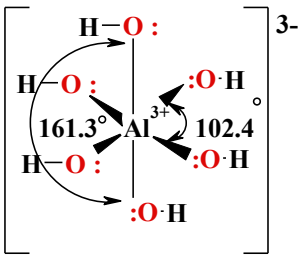
C Carbon
H Hydrogen
O Oxygen
N Nitrogen
P Phosphorus
Fe Iron

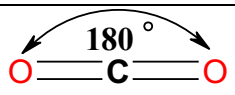
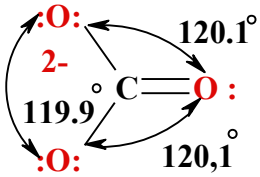
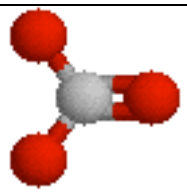
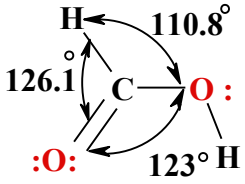
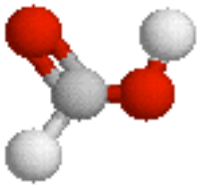
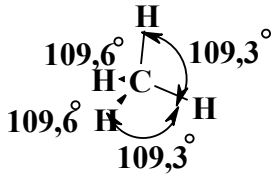
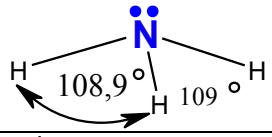
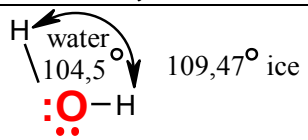
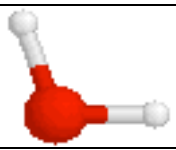
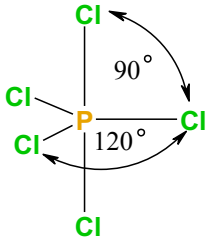
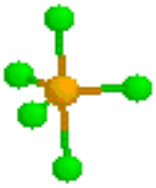
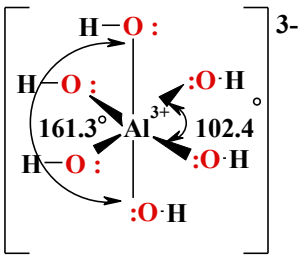
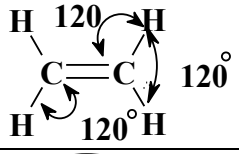
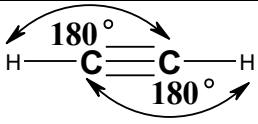
3. To investigate the 10 given molecular structures of compounds : **carbon(IV)oxide** CO_2, **carbonate anion** CO_3^{2-}, **formic acid** $HCOOH$, **methane** CH_4, **ammoniac** NH_3, **water** H_2O, **phosphoric penta chloride** PCl_5, **hexa hydroxo aluminate(III) anion** $[Al(OH)_6]^{3-}$, **ethene** $H_2C{=}CH_2$ and **ethyne** $HC{\equiv}CH$

Draw and Write into application table columns 1., 2., 3., 4., 5.:

1. first column molecular formula, chemical element content formula, molar mass and ISISDraw menu: Chemistry: generate Name of compound;
2. second column call the geometry figures and symmetrisation (hybridization) type; select: Mouse Click Action: Angle,.....
3. third column perspective ISIS Draw pictures and measured valence angles;
4. fourth column molecule model pictures in Ball and Stick mode;
5. fives column write the measured distances between atoms in **Å** angstroms.

with right mouse button use MDL options .....
menu: select: Mouse Click Action: Distance, ...

Molecular & Content formula Molar mass Name	geometry figure names symmetrisation hybridization σ,π bonds	**perspective pictures ISIS Draw valent bond Angles**	**molecule model pictures Ball and Stick mode**	measured **distances** between atoms in **Å angstroms**
$[Al(OH)_6]^{3-}$ H_6O_6Al 129,03 g/mol Hexa hydroxy aluminate (III) anion	**Octahedral Hexagonal Bipyramidal sp^3d^2**			**O-H Å** **O-Al Å**

Molecular & Content formula Molar mass Name	geometry figures and hybridization σ,π bonds	perspective pictures ISIS Draw valent bond Angles	molecule model pictures Ball and Stick mode	measured distances between atoms in Å angstrems
carbone(IV) oxide CO_2 44,01 g/mol	lineare sp 2σ 2π			1,498 Å
carbonate anions CO_3^{2-} 62,03 g/mol	trigonal planar sp^2 3σ 1π			1,296 Å 1,294 Å
formic acid HCOOH 129,03 g/mol	linear sp^2 4σ 1π			1,111 Å 1,205 Å 1,344 Å
metane CH_4 16,04 g/mol	tetragonal tetrahedral sp^3 4σ ; 0π			1,111 Å
amoniak NH_3 17,03 g/mol	trigonal piramid sp^3 3σ ; 0π			0,997 Å
water H_2O 18,02 g/mol	bent V-shape sp^3 2σ ; 0π			0,940 Å
phosphor pentachloride PCl_5 208,24 g/mol	trigonal piramid sp^3d 5σ ; 0π			2,076 Å 1,968 Å
$[Al(OH)_6]^{3-}$ H_6O_6Al 129,03 g/mol Hexa hydroxy aluminate (III) anion	Octahedral Hexagonal Bipyramidal sp^3d^2			1,665 Å 1,009 Å O-H 1,660 Å O-Al
etene $H_2C=CH_2$ 28.05 g/mol	trigonal planar sp^2 3σ ; 1π			1,330 Å 1,328 Å
etyne $HC\equiv CH$ 26.04 g/mol	linear sp 2σ ; 2π			1,212 Å 1,212 Å