Name: _____
Class: _____

Chemical Bonding Worksheet

Warm-Up Questions:

Watch the Khan Academy videos on molecular and ionic compound structure and properties.

1) Using Lewis symbols, diagram the reaction between magnesium and oxygen atoms to give the ionic substance MgO.

2) How many electrons are transferred?

3) Which atom loses electrons in the reaction?

Example #1:

Draw the electron configuration and Lewis electron dot symbol for the following elements listed in the table below.

Element	Electron Configuration	Lewis Symbol
Lithium		
Carbon		
Nitrogen		
Aluminum		
Chlorine		

Example #2:

Draw the Lewis structure for phosphorus trichloride, PCl_3 and show your work after each of the five steps.

Computational Exercise #1:

Take a screenshot of your optimized structure of PCl_3 including atom labels and any important bond distances or angles. Choose the ball-and-stick representation styling tool.

Example #3:

Analyze the structure of dichlorodifluoromethane, or CCl_2F_2 by 1) drawing the Lewis structure, 2) performing a geometry optimization using Maestro, and 3) measuring the bond lengths and bond angles listed below. Use the same DFT method as the last example (B3LYP-D3/6-31G**).

Lewis-Dot Structure of CCl_2F_2	Optimized Geometry of CCl_2F_2 using DFT	Bond Measurements from Optimized Geometry
		• C–F length: • C–Cl length: • F–C–F angle: • Cl–C–Cl angle: • Cl–C–F angle:

Example #4:

Determine the electronegativity differences and bond types of the following fluorine-containing compounds.

	F_2	HF	LiF
ΔEN			
Type of Bond			

Computational Exercise #2:

Now we will calculate the electrostatic potential surfaces of F_2, HF, and LiF to help us visually identify a chemical bond type. ESP maps will show the electron-density distribution on the surface of the molecules. This exercise involves four parts:

1) Build the molecules and minimize their geometries
2) Generate surfaces of the molecules
3) Map the electrostatic potentials to the molecular surfaces
4) Label each atom with electrostatic potential values

Individual Exercise:

Determine the electronegativity differences between the following hydrogen halides. Then generate an electrostatic potential surface for each molecule and identify any differences. For the single point calculations, use the following method:

- Theory: B3LYP-D3
- Basis Set: LACVP++**

Hydrogen Fluoride, H–F	Hydrogen Chloride, H–Cl
ΔEN =	**ΔEN =**
ESP Surface:	**ESP Surface:**

Hydrogen Bromide, H–Br	Hydrogen Iodide, H–I
ΔEN =	**ΔEN =**
ESP Surface:	**ESP Surface:**