RECOMMENDATIONS FOR THE REPORT FOR THE IONIC BONDING MODELING EXPERIMENT

In this modeling experiment you used a spreadsheet to build a model of the ionic bonding of NaCl-type compounds. Once you model was build you tested it by using it to model KCl and comparing your results to those done by your instructor and to the values listed in your laboratory manual. Once validated, you then used your spreadsheet to model the ionic bonding for one or more other NaCl-type compounds. In each case your model was also used to predict physical properties of these compound that one can relate directly to the nature of the ionic bond.

Your report should describe to the reader how your model was constructed, how it was validated, and about the new results you were able to generate. The following recommendations should help you with this task.

E - r and F - r Curves

- Your spreadsheet generated E - r and F- r curves for each material. Each graph showed the attractive and repulsive components and the total lattice energy and force. Copy these graphs to you report and format them using a style similar to that used in your text book. Here are a few suggestions:
- Each graph should be the same size and use the same scaling. This will make it much easier for the reader to compare the results for each series of calculations.
- Use caption styles similar to those used in your text book. Do not use the default titles and subtitles your spreadsheet uses. These are more appropriate for posters and presentations.
- Number each figure sequentially. The first figure in your report should be the first one mentioned in the text of your report, the last figure the last one referenced in the text.

Tables

In the course of your modeling efforts you generated a table of results of such things as the equilibrium lattice energy and atomic spacing, elastic moduli and other properties. If you tidy up this table a bit you can copy it to your report. This table will make it easy for the reader to find critical results and for you to write the report. Here are a few suggestions to help you generate this table:

- Create the table in a spreadsheet first, then copy-paste it into your report.
- Use standard table captions. These are located above the table and start out with “Table 1...” and then describe the table’s contents.
- Use notes at the bottom of the table to explain anything unusual.
- Don’t forget to include the units for each property.

Comparisons to Reference Data

Ideally your table will contain the calculated results, the corresponding reference values and even the percent difference between them. This will make it very easy to construct bar charts that illustrate the agreement between your calculations and those published in the literature. (See figure 1.) Here are a few suggestions to help you with these graphs.

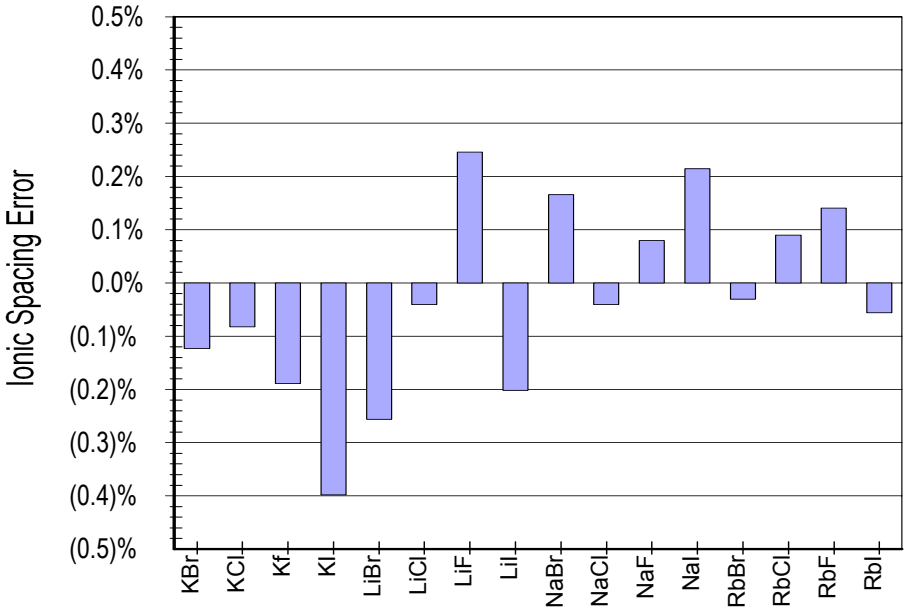

Figure 1 Bar chart illustrating the differences between the calculated and reference atomic spacings that corresponds to the minimum lattice energy of several NaCl-type compounds. (Note: the use of parentheses in the labels of the y axis is not recommended. This style is commonly used for business applications. The spreadsheet used to generate this figure forced this style.)

- Plan your chart. Bar charts are generally fairly simple but can become very confusing if you try to do too much with them. If you plan to illustrate the results of different calculations (lattice energy, density, melting point, etc.) for different compounds in the same chart think about how they can best be grouped.
- If you use more than one bar chart to represent your results then use the same style, size, etc. for each.
- One way of putting several figures in the same page in your report is to create a table and insert one chart into each cell in the table. For example, using a 2 x 2 table and help you organize and display four charts. Add a third row to the bottom of this table, join the cells so that it is as wide as the table, and enter your figure caption. Finally, turn off the cell boundaries so that the reader cannot tell that you even used a table structure.
- Use the same presentation guidelines and numbering system as you used for the E -r and F - r graphs.

Broader Issues

The discussion section of your report is where you interpret the data and derive deeper meaning from them. This experiment focuses on a fundamental aspect of all materials, specifically, the nature of the chemical bond and its relationship to various properties. Once you have dealt with the obvious interpretations of the immediate results, pause to consider this and any broader issues that may apply. Here are a few questions you might consider:

- Of all of the variables involved in your model, which of them determines the differences you observed when modeling different NaCl-type compounds?

- Do you think your model would work for all of the monovalent NaCl-type compounds listed in your laboratory manual?
- Could you use your spreadsheet to model the ionic bonding of divalent NaCl-type compounds such as MgO? Explain.
- Could you use your spreadsheet to model other, non-NaCl, type ionic compounds? If so, what would you have to do differently?
- Does this modeling experience help you to understand the origins of the macroscopic properties we are all familiar with, such as density, melting points, and elastic moduli?
- Do the broadly defined concepts of attractive and repulsive forces apply to metallic and covalent materials? If so, what lessons learned here can you translate to those materials?