

PREPARATION FOR THE IONIC BONDING MODELING EXPERIMENT

This simple exercise is designed to familiarize you with a few of the basics of ionic bonding and with spreadsheet programming before you come to the laboratory to tackle the full ionic bonding modeling project. While it involves only one of the equations used to represent ionic bonding it will give you a chance to get some experience entering data, writing simple equations, and formatting cells, three of the most basic skills required when using spreadsheets.

The Assignment

In this assignment you will perform some preliminary calculations of the lattice energy of three of NaCl-type materials. Once you have completed this assignment you should be ready to tackle the larger ionic bonding modeling project. You may even be able to reuse parts of this spreadsheet. If you don't complete this assignment it is very unlikely that you will be able to complete the full modeling project during the laboratory session.

Calculate the following:

- The equilibrium atomic spacing for the following compounds: KCl, RbF and LiI. Base these calculations on the values of the lattice constants listed in table 1 in the ionic bonding section of your laboratory manual.
- The minimum lattice energy (equation 4 in the laboratory manual) for the above compounds. Express the results in units of eV.
- The density for each compound. Express the results in units of Mg/m³.

Check your results against the values listed in your laboratory manual. Optionally, create a bar chart that illustrates the differences between your reference values and calculated results.

Print out your spreadsheet so that it fits on one page. This printout is due at the beginning of the laboratory session.

The Spreadsheet

Your spreadsheet should be written using the style recommended in your laboratory manual. The final results should look similar to a data sheet containing all essential information and which another person can easily read and understand. It should also be written in such a way that it can be easily expanded to include the calculations for all 16 compounds listed in your laboratory manual.

Figure 1 shows what your spreadsheet might look like. The major sections of this spreadsheet are described below. Your spreadsheet should contain each of these sections.

Header	Include the file name, your name, date and similar information at the top of the spreadsheet. This information is very helpful in managing your work, and it is standard practice in many engineering activities, for instance, on design drawings.
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Conversion Factors

Define all conversion factors in the next section. The function and importance of this section is similar to the “Physical Constants” section.

Physical Constants

Define all needed physical constants in a section that is separate from the calculations. This will make writing your equations much easier. This step is similar to standard programming practice where one must define all parameters, particularly constants, before writing the main body of code. Hint: make sure you enter the values of the physical constants in their full precision.

Materials Parameters

This section will contain entries for the materials parameters used by your equations. Include appropriate labels and any other text, such as units, that make it easier to understand what is being done.

Calculations This section you will perform the calculations. Each step in the calculations should be performed in a separate cell.

Results The last section will consist of the final results that you were after. Often this section simply refers to cells in the body of the spreadsheet, but it is always organized in such a way that the reader can clearly find and understand the results.

Quattro Pro 10 - [C:\Docu... \Preparation for the Ionic Bonding Experiment.qpw (unmodified)]

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Practice:A1 @ {} File:

1	File:	Preparation for the Ionic Bonding Experiment.qpw									
2	Owner:	Mike Meier									
3	Created:	January 4, 2003									
4	Revised:	March 21, 2003									
5	Description:	Practice calculations of ionic bonding energies, equilibrium spacing and density of NaCl-type compounds.									
6											
7	Conversion Factors	Physical Constants									
8	To convert from	To	Multiply by	Avogadro's Number: 6.022E+23 per mole							
9	Joules	eV	6.242E+18	Proton Charge: 1.602E-19 C							
10				Permittivity: 8.854E-12 C ² /Nm ²							
11											
12	Material Parameters	Calculations									
13	Substance:	KCl	RbF	LiI	Equilibrium Spacing: 0.3146 0.0000 0.0000 m						
14	Mineral Name:	Sylvite			Equilibrium Lattice Energy: -1.149E-18 ERR ERR Joules						
15	Lattice Parameter:	0.629170		nm	Mass of Unit Cell: 4.952E-22 0.000E+00 0.000E+00 g/unit cell						
16	Coordination Number:	6			Volume of Unit Cell: 0.2491 0.0000 0.0000 nm ³						
17	Number of Cations:	4		per unit cell	Density: 1.988E-21 ERR ERR g/nm ³						
18	Number of Anions:	4		per unit cell							
19	Valence of Cation:	1			Results						
20	Valence of Anion:	-1			Reference Lattice Energy: -7.190 0.000 0.000 eV						
21	Atomic Weight of Cation:	39.0983		g/mole	Calculated Lattice Energy: -7.171 ERR ERR eV						
22	Atomic Weight of Anion:	35.453		g/mole	Difference: -0.27% ERR ERR						
23	Madelung Constant:	1.747565			Reference Density: 1.988 0 0 Mg/m ³						
24	Repulsive Energy Coefficient:	2132.5		eV	Calculated Density: 1.988 ERR ERR Mg/m ³						
25	Repulsive Range Parameter:	0.0326		nm	Difference: 0.01% ERR ERR						
26	Reference Lattice Energy:	-7.190		eV							
27	Reference Density:	1.988		Mg/m ³							
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Practice Reference Modeling Constant Thermodynamics E F G H I J K L M N O P Q R S T U V W X Y Z

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Figure 1 Screen shot of the spreadsheet created for this assignment.