Examination # 2 Date: 09/30/96

Bonding Name: _____

ID #: _____

Question #1 (25 points) Organization of the information and clarity are both critical.....

Compare and contrast the bonding in crystalline materials. In your discussion, **which must be restricted to one page**, make sure you bring up the following concepts: bond directionality, lattice or cohesive energy, melting point, compressibility, dipoles, orbitals, covalent, polar, metal, molecular crystals, ionic solids, covalent solids and the appropriate examples.

Question #2 (25 points)

2.a (5 points)

Explain why bonds are not made by combining orbitals that are orthogonal to each other.

2.b (5 points)

What do we mean when we say "the bonding orbital is less bonding than the antibonding orbital is antibonding" ?

2.c (5 points)

In H, He^{+}, Li^{2+}, Be^{3+} the energy of a 2s electron is identical to that of a 2p electron. In atoms such as N, O or F this is no longer the case. Explain the above statements.

2.d (5 points)

Rank the following interactions in terms of their range of interaction from the shortest to the longest range and justify your answer. A) ion - ion B) rotating dipole - rotating dipole C) ion - dipole D) induced dipole - induced dipole

2.e (5 points)

$$U_{tot} = \sum_i \sum_j U_{ij} = N\left(z\lambda . \exp\left(\frac{-R}{\rho}\right) - \frac{\alpha q^2}{4\pi\varepsilon_0 R}\right)$$

Explain the physical meaning of all the terms involved in this equation and state what this equation is used for and what you learn from it. Write on the back if necessary.

Question #3 (25 points)

Butadiene has the following shape (shape was given):

a) Explain what this tells you about the state of hybridization of each of the carbon atoms (10 points).

b) Show (for 7 points) that the secular determinant for butadiene in the context of the Huckel Approximation is given by:

$(\alpha\text{-}E)^4 - 3\,(\alpha\text{-}E)^2\,\beta^2 + \beta^4$

c) Draw the Molecular Energy Diagram for the LCAO - MOs formed from the 2p electron(s) supplied by each of the carbon atoms and determine the energy associated with each MO (8 points)

Question #4. (25 points, 5 points each)

In all following questions, you must justify your answers with appropriate equation(s) and / or wording to get full credit.

a) Which of the following two bonds is the strongest and why CN^- or F_2^+ ?

b) Why is $\phi(1sH(A)) + \phi(1sH(B))$ a bonding orbital and $\phi(1sH(A)) - \phi(1sH(B))$ an antibonding orbital ? Hint: 1sH(A) is the 1s atomic orbital associated with the first H atom, and 1sH(B) corresponds to the second H atom in the H_2 molecule.

c) Show that the width of the band made from an infinite number of 2s orbitals is given by 4β , and that there is essentially no difference in energy between sucessive energy levels in the band. The solution of the secular determinant for a number N of 2s atomic orbitals is of the form $E_k = \alpha + 2\beta \cos(k\pi/N+1)$ for k = 1, 2 , ... N

d) How would you expect the melting point to vary in the series Ne, Ar, Kr, Xe ?

e) How would you expect the melting temperature to vary in the following series: Li_2 LiI LiBr LiCl Li F. Justify your answer.