CHAPTER 6

Tables

These tables are from

Understanding the properties of matter

by Michael de Podesta.

Table 6.1 Values of the lattice sums A_6 and A_{12} for three crystal structures. The bottom line of the table shows the cohesive energy U for each crystal structure calculated in terms of A_6 and A_{12} according to Equation 6.25.

	Simple cubic	**Body-centred cubic**	**Face-centred cubic**
A_6	8.4	12.25	14.45
A_{12}	6.2	9.11	12.13
Cohesive energy, U	-5.69ε	-8.24ε	-8.61ε

Table 6.2 Values of the lattice constant r_o and the cohesive energy per atom u calculated according to Equations 6.23 and 6.25 are compared with experimental values for neon, argon, krypton, and xenon. The values of σ and ε for each substance have been deduced from measurements in the *gaseous* phase of each substance by observing the deviations from perfect gas behaviour.

	Substance			
	Ne	**Ar**	**Kr**	**Xe**
$\sigma \times 10^{-10}$ m	2.74	3.44	3.65	3.98
$r_o(=1.09\sigma) \times 10^{-10}$ m	2.99	3.71	3.98	4.34
r_o(expt) $\times 10^{-10}$ m	3.13	3.75	3.99	4.33
Ratio(theory/expt)	0.955	0.989	0.997	1.002
$\varepsilon \times 10^{-3}$ eV	3.1	10.3	14.0	20.0
$u = -8.6\varepsilon \times 10^{-3}$ eV	–27	–89	–120	–172
u(expt) $\times 10^{-3}$ eV	–20	–80	–110	–170
Ratio(theory/expt)	1.35	1.11	1.09	1.01

Table 6.3 The first few energy levels for particles trapped in a box. The columns show (i) the quantum numbers of the states, (ii) the energy of the states in units of $h^2/8mL^2$, for example $E(1,1,3) = A[1^2 + 1^2 + 3^2] = 11A$ where $A = h^2/8mL^2$, (iii) the number of quantum states with the same energy, (iv) the number of electrons that can be accommodated at that energy, and (v) the running total of the number of electrons able to be accommodated with energy equal to or less than the current energy, i.e. the running total of column (iv).

Quantum numbers n_x, n_y, n_z	Energy in units of $h^2/8mL^2$	Number of states	Number of electrons able to be accommodated with this energy (including spin)	Number of electrons able to be accommodated with energy less than or equal to the current energy
(1,1,1)	3	1	2	2
(1,1,2) (1,2,1) (2,1,1)	6	3	6	2 + 6 = 8
(1,2,2) (2,1,2) (2,2,1)	9	3	6	2 + 6 + 6 = 14
(1,1,3) (1,3,1) (3,1,1)	11	3	6	2 + 6 + 6 + 6 = 20
(2,2,2)	12	1	2	2 + 6 + 6 + 6 + 2 =22
(1,2,3) (1,3,2) (2,1,3) (2,3,1) (3,2,1) (3,1,2)	14	6	12	2 + 6 + 6 + 6 + 2 + 12 = 34

Table 6.4 Evaluating the energy difference between options *A* and *B* in Figure 6.17 for eight electrons.

	Option A (separate atoms)	**Option B (metallic state)**
Energy of 8 electrons	$24 \times h^2/8ma^2$	$10.5 \times h^2/8ma^2$
Average energy per electron	$3 \times h^2/8ma^2$	$1.31 \times h^2/8ma^2$
Energy *difference* per electron	$-1.69 \times h^2/8ma^2$	

Table 6.5 Evaluating the energy difference between options *A* and *B* in Figure 6.17 for a free electron gas.

	Option *A* (separate atoms)	**Option *B* (metallic state)**
Energy of N electrons	$3N \times h^2/8ma^2$	$N \times 3E_F/5$
Average energy per electron	$3 \times h^2/8ma^2$	$3E_F/5$
Energy *difference* per electron	$3E_F/5 - 3h^2/8ma^2$	

Table 6.6 Summary of what has been considered and neglected in Chapter 6.

Bonding type	What we considered	What we neglected
Molecular	We calculated the cohesive energy of an array of neutral molecules interacting through fluctuations of their electric charge distribution.	We neglected to consider the origin of the charge distributions, and the origin of their fluctuations. These can only be properly calculated using quantum mechanics.
Ionic	We calculated the cohesive energy of an array of positive and negative ions interacting through the coulomb interaction.	We neglected to consider why electrons transfer themselves completely from one ion to another. This can only be understood by quantum mechanical calculations of the charge distribution around atoms and ions.
Covalent	We calculated the cohesive energy of a covalent bond in terms of a simple model of the charge distribution within the bond.	We neglected to consider *why* that particular charge distribution occurs. This can only be understood by quantum mechanical calculations of the electron wave functions near both atoms. Notice that in addition to the Coulomb energy which we calculated, there will be an additional 'delocalisation' term analogous to that which occurs on a larger scale in metals
Metallic	We calculated the cohesive energy of a metal by considering the change in energy of the wave functions as they were allowed to expand into a large volume.	We neglected to include the effects of the strong Coulomb interactions between electrons and other electrons, and between electrons and ions.