Problem set 2

Conor Redington

1. **a)** 12 **b)** 12 **c)** 8
2. **a)** 74% **b)** 74% **c)** 68%
3. 4 Ba^{2+}; 4 O^{2-}: The NaCI lattice is face centered cubic with 4 Sodium ions and 4 Chloride ions in each unit cell. If Barium Oxide has the same lattice structure then it should have 4 Barium ions and 4 Oxygen ions too.
4. **a)** left to right: (0, 0, 1), (1, 0, 0), (0, 1, 0)

   b) left to right: (1, 0, 1), (1, 1, 0), (0, 1, 1)

   c) left to right: $\{1, 1, 1\}$, $\{1, \bar{1}, 1\}$, $\{\bar{1}, 1, 1\}$
5. **a)** If the volume of the cell is $a^3 = (4.059 \times 10^{-8} cm)^3$ and $\rho = 2.431 g/cm^3$ then the $m_{cell} = a^3 * \rho = 1.6257 \times 10^{-22}$ which is approximately 97.9 amu subtracting the mass of Bromine from this leaves 18 amu. Looking up common cations, one that has a mass of 18 amu would be NH_4^+. So X could be Ammonium (NH_4^+).

   b) Where the diagonal of the unit cell has the diameter of the bromide ion ($2 * 1.96\dot{A}$) and the diameter (a radius at each corner) of the cation X. At room temp.

   $$(d_{br} + d_X)^2 = 2a^2 \rightarrow d_X = 1.82 \rightarrow r_X = O.91\dot{A}$$

   using the same line of thought then for it at the next temperature but changing the volume, because the rock salt structure has the same face.

   $$r_X = 2.896\dot{A}$$

6. **a)** Ni^{2+} has a valence shell of $3d^8$. Square planar are usually low spin, so it will populate levels from low to high (t_{2g} to e_g) Meaning all three t_{2g} orbitals are paired and then one e_g orbital is paired. 0 unpaired electrons; $\mu_b = 0$

   b) Ni^{2+} has a valence shell of $3d^8$. The stable orbitals will be populated by 4 electrons (paired) first. Then the next four will occupy the degenerate orbitals with some crystal field splitting d_{xy}, d_{xz}, d_{yz} leaving 2 unpaired orbitals. $\mu_b = 2.828$.

   c) Ti^{3+} has a valence shell of $3d^1$. It will populate 1 of the t_2g orbitals so n = 1. $\mu_b = sqrt3 = 1.73$.

   d) Mn^{+5} has a valence shell of $3d^5$. High spin would mean that all orbitals gets an unpaired electron. $\mu_b = \sqrt{5(7)} = 5.91$

   e) Low spin would imply that only the lower energy orbitals will be filled and pairing would occur on these before occupying the higher energy orbitals. This one leave one orbital unpaired. $\mu_b = 1$
7. **a)** Antimony has more valence electrons so it would be adding negative charges carriers: n-type.

   b) Aluminium has less valence electrons which acts as a postive carrier (hole): p-type.

c) Antimony in Tin oxide would be n-type.

d) Nitrogen in zinc oxide I'm not too sure that it would be either type, it might offer some other property.

8. **a)** $BaCO_3 + TiO_2 \rightarrow BaTiO_3 + CO_2$

   b) The molar mass of the reactants and products is

$$197.33g/mol + 79.8g/mol = 233.13g/mol + 44g/mol$$

100g of product is 0.43 moles of product. Multiply across by 0.43 moles to get 84.85g + 34.31g = 100g + 18.82g. 18.82 grams of by-product (CO2) would be generated.

c) Strontium is in the same group as Barium in the periodic table having a stable s orbital valence shell so I would expect it to have a similar structure in this reaction with the same by-product.