Chapter 1

1.1

(a) In water "ppb" refers to a mass fraction:

$$ppb(\text{water}) = \frac{\text{mass of contaminant} \times 10^9}{\text{mass of (water + contaminant)}}$$

In air "ppb" refers to a mole or, equivalently, volume fraction:

$$ppb(\text{air}) = \frac{\text{moles (or volume) of contaminant} \times 10^9}{\text{moles (or volume) of (air + contaminant)}}$$

Since the mass and moles of a contaminant are usually much lower than the mass of water and moles of air, respectively, the contaminant is usually left out of the denominator.

(b) 35 ppm is equal to $\frac{35 \times 10^{-6} \text{ moles CO}}{\text{mole air}}$

To convert this to a mass concentration, we first need to determine what volume is taken up by 1 mole of air. We can use the IDEAL GAS LAW:

$$PV = nRT \; ; \; \frac{V}{n} = \frac{RT}{P}$$

Assuming P = 1 atm and T = 293 K, and using $R = 82.05 \times 10^{-6} \frac{\text{atm m}^3}{\text{mol K}}$:

$$\frac{V}{n} = \frac{(82.05 \times 10^{-6} \text{ atm m}^3 \text{ mol}^{-1} \text{ K}^{-1})(293 \text{ K})}{1 \text{ atm}}$$

$$= 0.024 \text{ m}^3 \text{ mol}^{-1}$$

We also need to know what mass is contained in 1 mole of CO:

$$MW_{CO} = 12 \text{ g mol}^{-1} + 16 \text{ g mol}^{-1} = 28 \text{ g mol}^{-1}$$

Thus, the conversion is:

$$\left(\frac{35 \times 10^{-6} \text{ mol CO}}{\text{mol air}}\right)\left(\frac{28 \text{ g CO}}{\text{mol}}\right)\left(10^3 \frac{\text{mg}}{\text{g}}\right)\left(\frac{1 \text{ mol air}}{0.024 \text{ m}^3 \text{ air}}\right)$$

$$= \boxed{41 \text{ mg m}^{-3}}$$

(c) The conversion is:

$$\left(\frac{0.005 \text{ mg Cd}}{\text{L } H_2O}\right)\left(\frac{1 \text{ L } H_2O}{1000 \text{ g } H_2O}\right)\left(\frac{1 \text{ g Cd}}{10^3 \text{ mg Cd}}\right)(10^6) = \boxed{0.005 \text{ ppm}}$$

(10^6 — to convert to ppm)

1.2

(a) As in problem 1.1(b) above, we use the ideal gas law and the molecular weight of the contaminant, in this case $CHCl_3$, to make the conversion. Recall:

$$PV = nRT \; ; \quad \frac{V}{n} = \frac{RT}{P}$$

With $P = 1$ atm and $T = 293$ K, and using $R = 82.05 \times 10^{-6} \frac{\text{atm m}^3}{\text{mol K}}$:

$$\frac{V}{n} = \frac{(82.05 \times 10^{-6} \text{ atm m}^3 \text{ mol}^{-1} \text{ K}^{-1})(293 \text{ K})}{1 \text{ atm}}$$

$$= 0.024 \text{ m}^3 \text{ mol}^{-1}$$

The molecular weight of $CHCl_3$ is:

$$MW_{CHCl_3} = 12 \text{ g mol}^{-1} + 1 \text{ g mol}^{-1} + 3(35.5 \text{ g mol}^{-1})$$

$$= 119.5 \text{ g mol}^{-1}$$

The conversion is:

$$\left(\frac{0.4 \ \mu\text{g CHCl}_3}{\text{m}^3 \text{ air}}\right)\left(\frac{0.024 \text{ m}^3 \text{ air}}{\text{mol air}}\right)\left(\frac{1 \text{ g}}{10^6 \ \mu\text{g}}\right)\left(\frac{1 \text{ mol CHCl}_3}{119.5 \text{ g CHCl}_3}\right)(10^9)$$

$$= \boxed{0.08 \text{ ppb CHCl}_3}$$

(b) We use the fact that the density of water is 1 g/mL to make the conversion:

$$\left(\frac{42 \ \mu\text{g CHCl}_3}{\text{L H}_2\text{O}}\right)\left(\frac{1 \text{ L}}{10^5 \text{ mL}}\right)\left(\frac{1 \text{ mL H}_2\text{O}}{\text{g H}_2\text{O}}\right)\left(\frac{1 \text{ g}}{10^6 \ \mu\text{g}}\right)(10^9)$$

$$= \boxed{42 \text{ ppb CHCl}_3}$$

(c) The exposures to $CHCl_3$ through inhalation and ingestion:

	Inhalation	Ingestion
Amount consumed	20 m^3 day^{-1}	2 L day^{-1}
$CHCl_3$ concentration	0.4 μg m^{-3}	42 μg L^{-1}
$CHCl_3$ exposure	**8 μg day^{-1}**	**84 μg day^{-1}**

1.2 (continued)

(d) The exposures to C_2Cl_4 through inhalation and ingestion:

	Inhalation	Ingestion
Amount consumed	$20\ m^3\ day^{-1}$	$2\ L\ day^{-1}$
C_2Cl_4 concentration	$2.1\ \mu g\ m^{-3}$	$0.10\ \mu g\ L^{-1}$
C_2Cl_4 exposure	$42\ \mu g\ day^{-1}$	$0.20\ \mu g\ day^{-1}$

(e) Ingestion is more important than inhalation for chloroform (by a factor of 10), while inhalation is more important for C_2Cl_4.

1.3

(a) The conversion in water is:

$$\left(\frac{80\times10^{-9}\ g\ C_2H_3Cl}{g\ H_2O}\right)\left(\frac{10^6\ \mu g}{g}\right)\left(\frac{10^3\ g}{kg}\right)\left(\frac{1\ kg\ H_2O}{L\ H_2O}\right)$$

$$= \boxed{80\ \mu g\ L^{-1}\ C_2H_3Cl}$$

Note: In general, $[ppb] = \left[\frac{\mu g}{L}\right]$ in water.

(b) The conversion in air is:

$$\left(\frac{80\times10^{-9}\ mol\ C_2H_3Cl}{mol\ air}\right)\left(\frac{62.5\ g\ C_2H_3Cl}{mol}\right)\left(\frac{10^6\ \mu g}{g}\right)\left(\frac{1\ mol\ air}{0.024\ m^3}\right)\left(\frac{1\ m^3}{10^3\ L}\right)$$

$$= \boxed{0.2\ \mu g\ L^{-1}\ C_2H_3Cl}$$

Note: See problems 1.1 and 1.2 for a calculation of what volume is occupied by a mole of air. P = 1 atm and T = 293 K are assumed.

1.4

We want to convert mass concentration to molarity and normality for five ions in drinking water. Recall that the definitions of molarity and normality are as follows:

$$\text{MOLARITY} = M = \frac{\#\text{ of moles of solute}}{\text{Volume of solution}} - \left[\frac{mol}{L}\right]$$