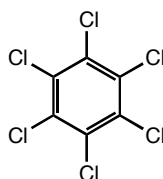


## Metals, Toxins, and Human and Environmental Health

These problems come from an environmental chemistry textbook and will need to be revised before they can be published

1. Hexachlorobenzene (HCB) was widely used after WWII as a fungicide for cereal crops. (reminder – the vertices represent carbons)



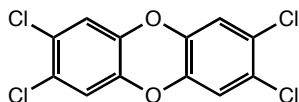
0.0062 mg of HCB dissolves in 1 L of water. Determine the molecular weight of HCB and determine how many moles per L of HCB dissolve in water.

HCB has a log Kow of 5.3 – If you had 1 mole of HCB and placed it in 1L of water and 1L of octanol, how much of the HCB would end up in the water and how much would end up in the octanol?

The LD50 is the dose needed to kill half the animals in the toxicity study. The LD50 for HCB is 3500-10000 mg/kg and for DDT it is 115 mg/kg. Which compound has greater acute toxicity? How many mg of DDT would be fatal to you?

The bioaccumulation factor (BCF) is the ratio of the concentration of a specific chemical in a fish relative to that dissolved in the surrounding water assuming that the fish is eating fairly low on the food chain. It can be approximated by the octanol-water partition coefficient. What therefore would the predicted concentration of HCB be in the fat of a fish that swims in waters containing 0.0000010 ppm of HCB?

2. Dioxin is a name given to a series of structurally related compounds that form as unwanted byproducts in the syntheses of many pesticides.



2,3,7,8-TCDD (2,3,7,8-tetrachlorodibenzo-p-dioxin)

Agent Orange was a 1:1 mixture of two compounds (2,4-dichlorophenoxyacetic acid 2,4-D and 2,4,5-trichlorophenoxyacetic acid 2,4,5-T) widely used in the Vietnam war as a defoliating agent. The synthesis of 2,4,5-T is known to produce dioxins and Agent Orange was contaminated with dioxin levels of about 20 ppm. Dioxins are also found in very small amounts as outputs from fires, including incinerators. For this reason, incineration of chemicals that contain chlorines are highly regulated.

Below is a table of the average dioxin content in the American food supply

Food	Dioxin concentration in picograms/g	Average dioxin intake (pg/person/day)
Ocean fish	500	8.6
Meat	35	6.6
Cheese	16	0.31
Milk	1.8	0.20

Assume that the average person has about 32 pp trillion of 2,3,7,8-TCDD in her fat and is at steady state. Determine the residence time of TCDD in humans.

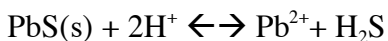
The LD50 for dioxin in a range of animals is given below:

Species	Route	LD50 (mg/kg)
Guinea pig (male)	Oral	0.6
Guinea Pig (female)	Oral	2.1
Rabbit	Oral	115
Rabbit	Dermal	275
Monkey (female)	Oral	<70
Rat (female)	Oral	22
Rat (female)	Oral	45-500
Mouse (male)	Oral	<150
Dog (male)	Oral	30-300
Dog (female)	Oral	>100
Frog	Oral	1,000
Hamster	Oral	1157

Scientific American 1986, 254, 29-35.

What do you think the LD50 is for humans? How would you determine it? What other aspects of dioxin toxicity might be of interest? Describe how you would assess dioxin's toxicity in one other area of interest.

- Galena, the dominant lead-containing ore, dissolves in water to form  $\text{Pb}^{2+}$  and  $\text{S}^{2-}$ .  $\text{S}^{2-}$  quickly reacts with available protons ( $\text{H}^+$ ) to form  $\text{H}_2\text{S}$  so the overall reaction for the dissolution of galena in water can be written as:



Write the expression for the equilibrium constant.

Given that the equilibrium constant is  $6.5 \times 10^{-8}$ , calculate the  $\text{Pb}^{2+}$  concentration when  $\text{pH} = 1$  and  $\text{pH} = 10$ . What does this information tell you about the conditions in which lead in water is likely to be most problematic?