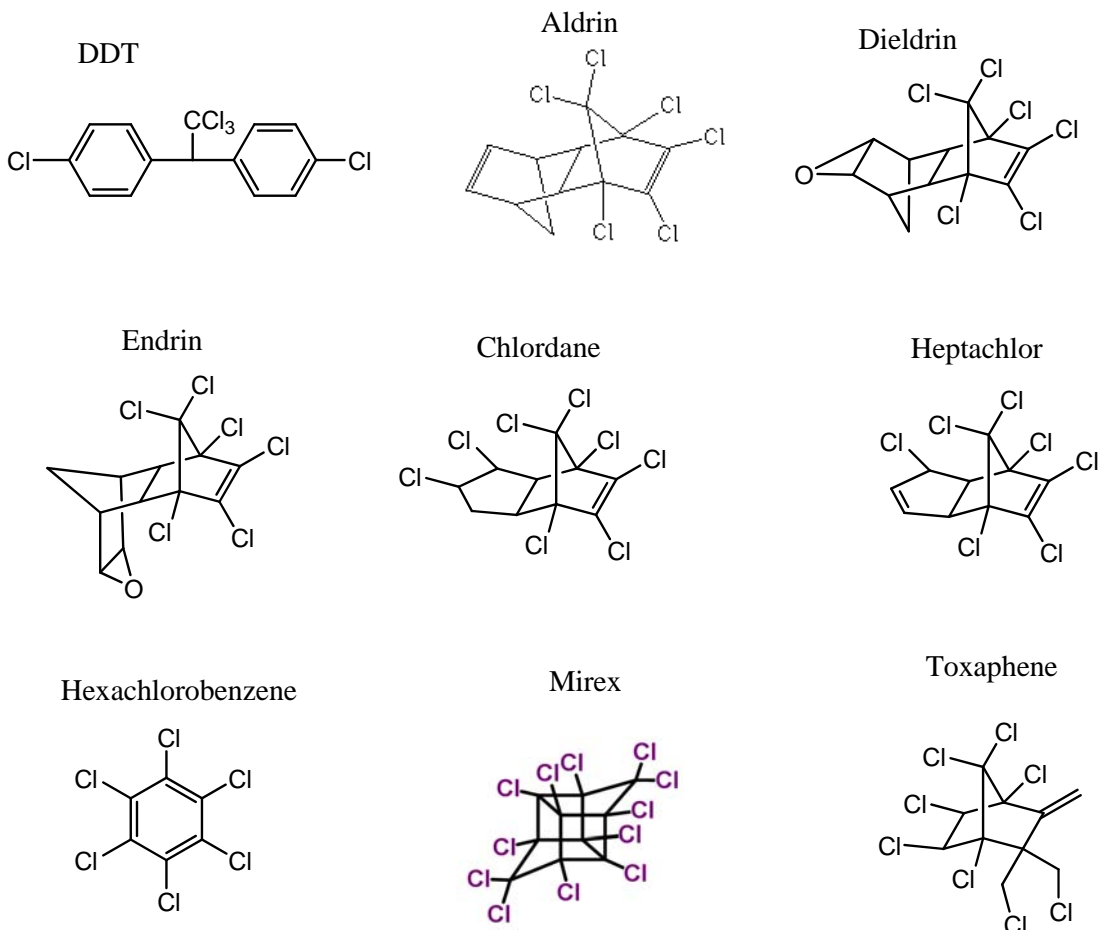


Green Chemistry Homework problem answers:

1. Find the structure of at least three of the POPs given in Table 13-2. What is the common structural feature in these compounds? Are any or all of them legal to use currently in the US? Cite the source for your information—please NEVER use Wikipedia.



These compounds share a heavily chlorinated structure, most often containing bicyclic or polycyclic structures (or aromatic rings)

DDT—banned in US in 1973-- <http://www2.epa.gov/aboutepa/ddt-ban-takes-effect>

Aldrin—banned in US--<http://www.popstoolkit.com/about/chemical/aldrin.aspx>;

[http://scorecard.goodguide.com/chemical-groups/one-list.tcl?short\\_list\\_name=brpest](http://scorecard.goodguide.com/chemical-groups/one-list.tcl?short_list_name=brpest)

Dieldrin—most uses banned in 1987--<http://www.epa.gov/pbt/pubs/aldrin.htm>

Endrin—most uses banned in 1980--

<http://water.epa.gov/drink/contaminants/basicinformation/endrin.cfm>

Chlordane—Banned in 1983 (except for termites)--

[http://nlquery.epa.gov/epasearch/epasearch?querytext=chlordane&fld=ttnatw01&area name=Technology+Transfer+Network+Air+Toxics+Web+Site&areacontacts=http%3A%2F%2Fwww.epa.gov%2Ftn%2Fatw%2Fcontact.html&areasearchurl=&result\\_template=epafiles\\_default.xsl&filter=sample4filt.hts](http://nlquery.epa.gov/epasearch/epasearch?querytext=chlordane&fld=ttnatw01&area name=Technology+Transfer+Network+Air+Toxics+Web+Site&areacontacts=http%3A%2F%2Fwww.epa.gov%2Ftn%2Fatw%2Fcontact.html&areasearchurl=&result_template=epafiles_default.xsl&filter=sample4filt.hts)

Heptachlor—insecticide banned in all food products in 1978, banned from seed treatment in 1983--

[http://nlquery.epa.gov/epasearch/epasearch?querytext=Heptachlor&fld=ttnatw01&areaname=Technology+Transfer+Network+Air+Toxics+Web+Site&areacontacts=http%3A%2F%2Fwww.epa.gov%2Fttn%2Fatw%2Fcontact.html&areasearchurl=&result\\_template=epafiles\\_default.xml&filter=sample4filt.hts](http://nlquery.epa.gov/epasearch/epasearch?querytext=Heptachlor&fld=ttnatw01&areaname=Technology+Transfer+Network+Air+Toxics+Web+Site&areacontacts=http%3A%2F%2Fwww.epa.gov%2Fttn%2Fatw%2Fcontact.html&areasearchurl=&result_template=epafiles_default.xml&filter=sample4filt.hts)

Hexachlorobenzene—banned as a pesticide in 1984--

<http://www.toxipedia.org/display/toxipedia/Hexachlorobenzene;>  
<http://pmep.cce.cornell.edu/profiles/extoxnet/haloxyfop-methylparathion/hexachlorobenzene-ext.html>

Mirex—banned in 1978--<http://www.epa.gov/pbt/pubs/mirex.htm>

Toxaphene Banned since 1990-- <http://www.epa.gov/ttnatw01/hlthef/toxaphen.html>

There are many good websites for data, but I like the EPA site, since they are most involved in regulation therefore most up to date and reputable (?)

2. Everything is toxic; it is all a question of dosage. Find the LD<sub>50</sub> values for the following compounds around the house: Bleach, gasoline, acetaminophen, capsaicin (from hot peppers!) and Windex. Calculate how much Windex you would need to ingest to reach the LD<sub>50</sub> dosage. You may assume the Windex has the same density as water. Please convert this value into cups, to give yourself a good visualization.

Bleach: LD<sub>50</sub> (oral mouse) 5800 mg/kg

Gasoline: LD<sub>50</sub> (oral rat) 18.75 mL/kg ~ 13,000 mg/kg

Acetaminophen: LD<sub>50</sub> (oral rat) 1900 mg/kg

Capsaicin: LD<sub>50</sub> (oral mouse) 47.2 mg/kg

Windex: LD<sub>50</sub> (oral mouse) 5000 mg/kg

Estimate 150 lb person:

$$150 \text{ lb} * (1 \text{ kg} / 2.2 \text{ lb}) * (5 \text{ g Windex} / \text{kg}) * (0.996 \text{ g} / \text{mL}) * (1 \text{ cup} / 236.59 \text{ mL}) \\ = 1.44 \text{ cups}$$

3. Why would Harpin (a pesticide, section 2.16) not be expected to accumulate in the environment in the same way that many other pesticides do?

Harpin is a bacterial protein, and is normally found in many plant cells (not a non-native compound). The wastes from the synthesis of this compound are biodegradable. Being a natural product it is highly sensitive to degradation, it is rapidly decomposed by microorganisms in the soil, and by UV light from the sun, therefore it will not accumulate in water or biomass

4. a) The first dry cleaning solvents were gasoline and kerosene. What are the hazards associated with these solvents? b) PERC replaced these chemicals as a popular solvent in the middle of the 20<sup>th</sup> century. What are the hazards associated with PERC? What advantage did it have over kerosene? c) Liquid CO<sub>2</sub> is now a popular replacement solvent for PERC. Does this new solvent have any associated hazards?

a) Gasoline and kerosene—both are highly flammable liquids with high vapor pressures; gasoline is a suspected carcinogen and both are associated with neurotoxic effects from long term exposures. b) PERC is not flammable, but tends to accumulate in the fat tissues. Short term exposure can cause nervous system problems, long term exposure can cause memory loss and confusion, liver and kidney damage, and cancer. As a gas, PERC can contribute to photochemical smog (but it tends to react quickly before reaching the upper atmosphere so it is not thought to damage the ozone layer). c) One of the biggest hazards of liquid CO<sub>2</sub> is the fact that it must be kept under pressure, therefore poses an explosion hazard. Large volumes released suddenly will displace air; therefore can be deadly via suffocation. It is often kept cold, which can lead to dangers of freezing damage to skin

5. Even though most ions have extremely high melting points, ionic liquids melt near room temperature. What are the features in ionic liquids which lead to this low mp? What are the advantages to using an ionic liquid in place of a typical organic as a solvent?

Ionic liquids usually utilize at least one ion (generally the cation) which is a large organic species where the charge is dispersed over a region (usually a resonating charge). The large size and diffusion of charge means that the cations and anions are poorly coordinated. Since they cannot form tight ion pairs, these systems usually have low melting points

Ionic liquids are not flammable, and they have extremely low vapor pressures (so little explosion hazard or VOC release). They are good at dissolving a variety of organic, inorganic, and polymeric materials, so less solvent can be used to dissolve things. They have a wide liquid range so can be used for high-temperature reactions, yet they resist oxidation like other organics would do at high temps.

6. Find an old reaction from lab—you may use your own data or find a current organic lab student and bribe them to share data with you. List the reagents, solvents, catalyst, products/byproducts for the reaction being performed. Calculate a theoretical yield for the reaction. Calculate atom economy for this reaction.

Many answers possible. Should utilize reagents consumed (not catalysts or solvents). For the most part, high theoretical yields in classical syntheses will still have low atom economies.