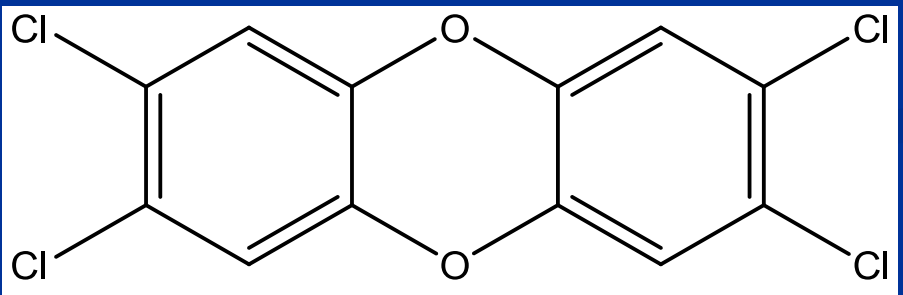
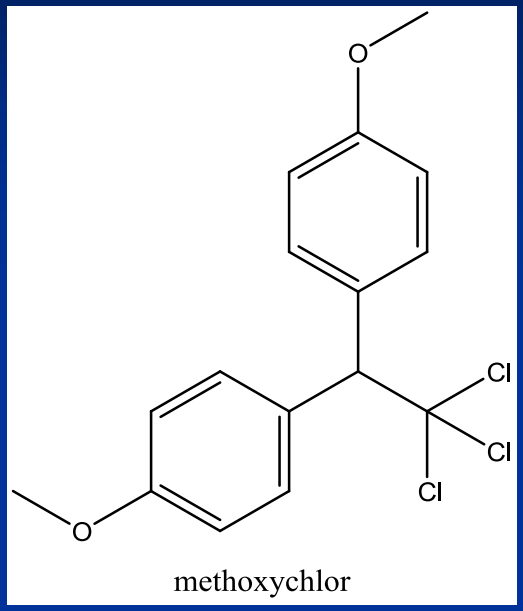
# Atom/Fragment approach

$$\log K_{i,ow}(25\ ^{\circ}C) = \sum_{k} n_k f_k$$



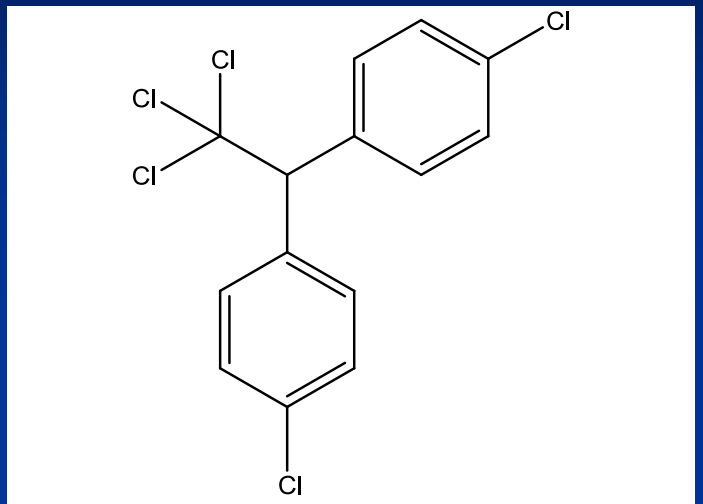

2,3,7,8-tetrachlorodibenzo-p-dioxin

# Fragments based on a related substance



methoxychlor

Based on DDT

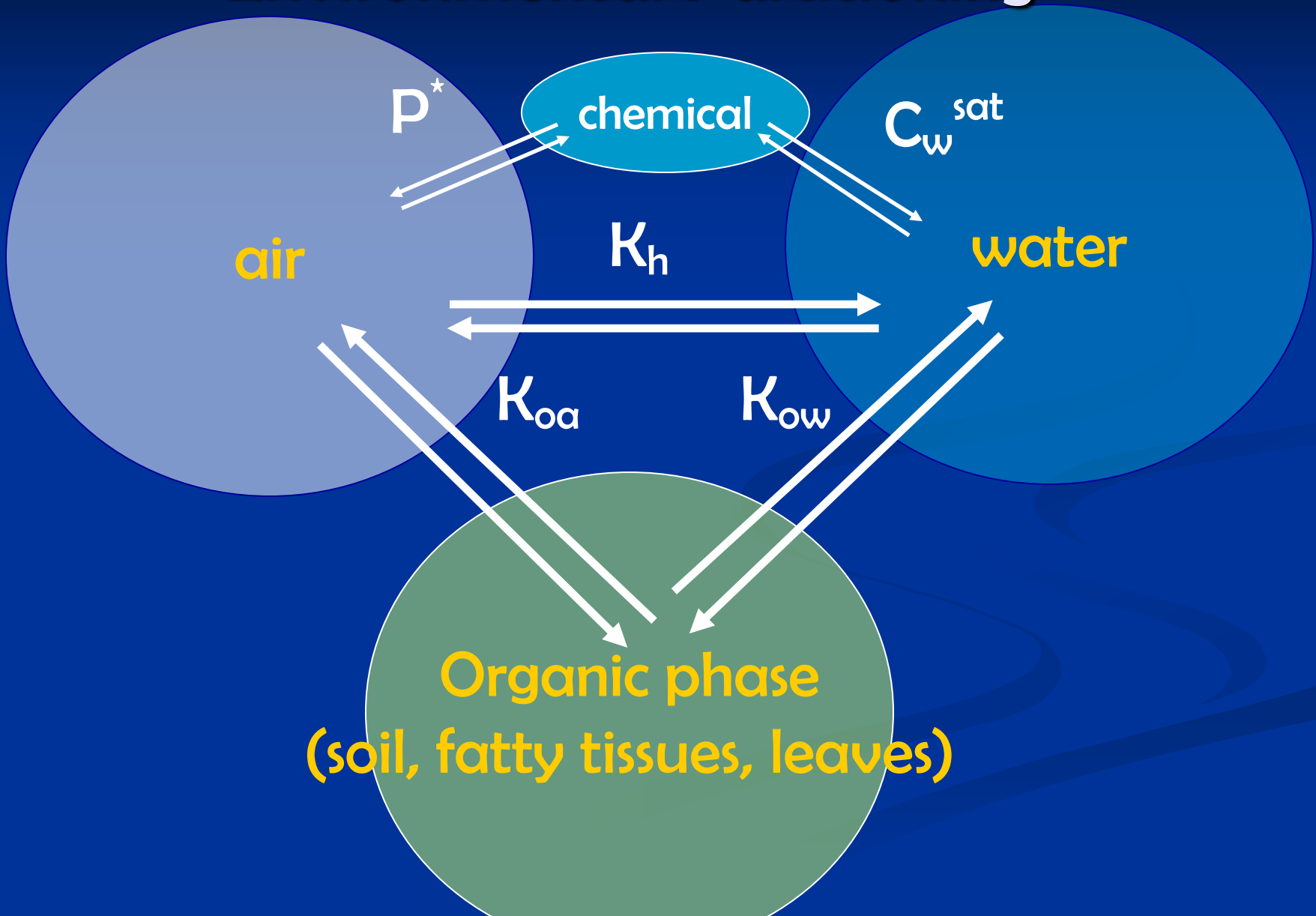


4,4'-(2,2,2-trichloroethane-1,1-diyl)bis(chlorobenzene)

log $K_{ow}$(25°C)=6.20

**First establish your intuition…do you expect methoxychlor's $K_{ow}$ to be greater or less than DDTs?**

# Environmental Partitioning



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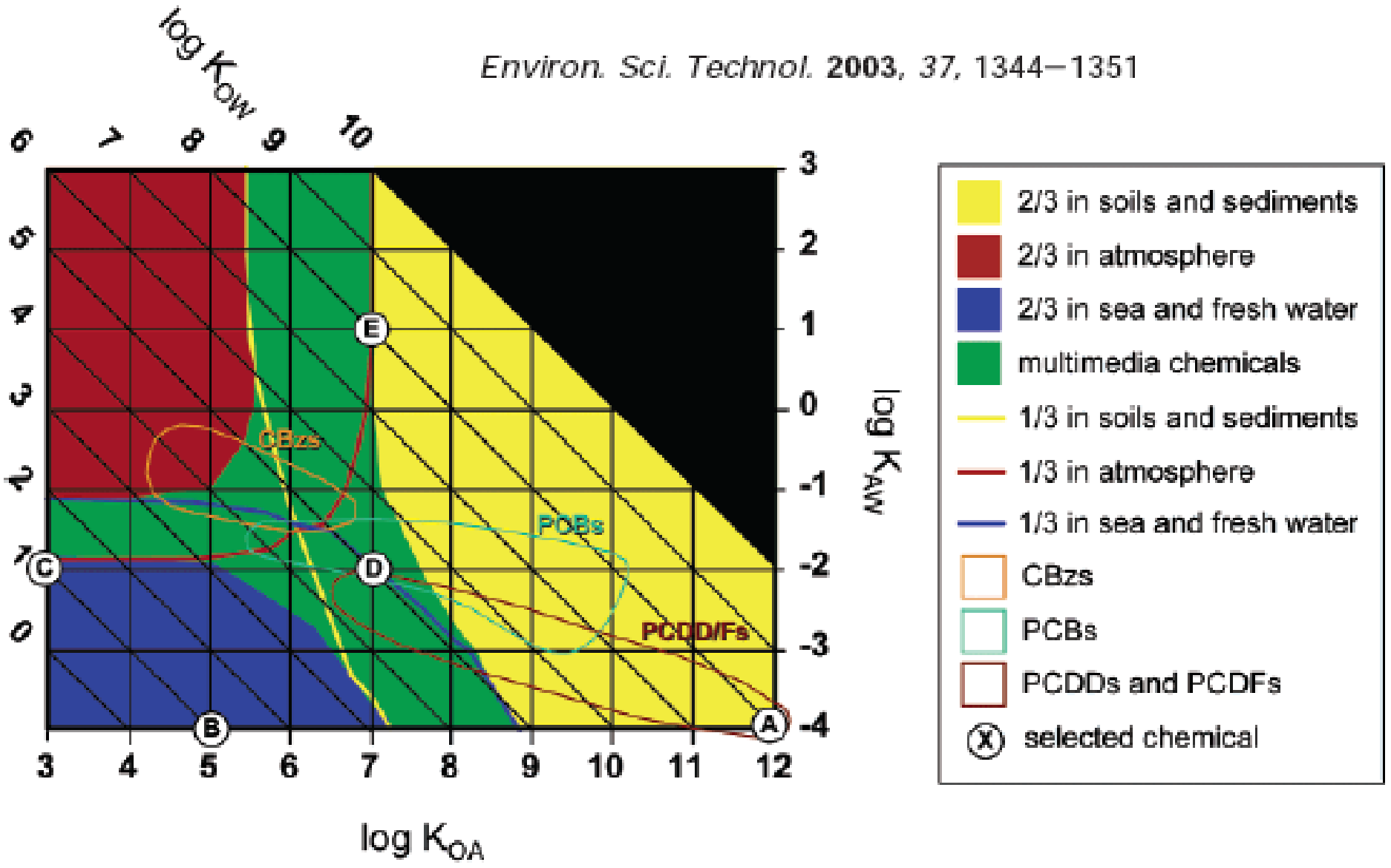


FIGURE 3. Primary environmental compartments for hypothetical chemicals defined by their partitioning properties log $K_{AW}$, log $K_{OA}$, and log $K_{OW}$. The distribution between media was calculated with the Globo-POP model assuming 10 years of steady emissions of perfectly persistent chemicals into air, water, and soil (1/3 each) using a zonal emission distribution matching that of the human population. Chemicals with a log $K_{OW}$ > 10 are unlikely to exist. The white circles locate the five chemicals used in the sensitivity analysis within that chemical space. Closed curves indicate the partitioning properties of the chlorobenzenes (CBzs), polychlorinated biphenyls (PCBs), polychlorinated dibenzo-*p*-dioxins (PCDDs), and dibenzofurans (PCDFs).