Distribution Ratio of Some Chlorinated Hydrocarbon Insecticides between Hexane and Water

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It is known that the solubility of chlorinated hydrocarbon insecticides in water is very low but not negligible. Organic solvents e.g. hexane are used for extraction of water solutions because the distribution ratios (organic solvent to water) are presumed to be very large. Little is known about their order of magnitude or their values in relation to each other.

This distribution ratio cannot be measured directly after shaking a hexane solution with pure water because the decrease of the concentration in the hexane layer is too low, and water cannot be injected into a gas-chromatograph without affecting the sensitivity of the electron-capture detector. Therefore it is necessary to extract the water layer again with pure hexane. A formula is given to calculate the distribution ratio and the results are discussed of the estimation of this value for lindane, aldrin, dieldrin, heptachlor, heptachlor epoxide and DDT.

Theory

If V_o ml hexane containing $V_o C_i$ µg insecticide is shaken

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with V_w ml water, an equilibrium is eventually reached in which

the concentrations are C_o and C_w µg per ml in the organic and

in the water layer, respectively. From the water layer, V_w' ml

is shaken again with V_o' ml fresh hexane. At equilibrium

$$V_w' C_w' + V_o' C_o' = V_w' C_w \quad \text{µg} \qquad (I)$$

in which C_o' and C_w' are the new equilibrium concentrations.

The distribution ratio K is independent of the concentration,

therefore

$$K = \frac{C_o}{C_w} = \frac{C_o'}{C_w'} \qquad (II)$$

By eliminating C_w and C_w' it follows that

$$K = \frac{V_w'}{V_o'} \cdot \frac{C_o - C_o'}{C_o'} \approx \frac{V_w'}{V_o'} \cdot \frac{C_i}{C_o'} \qquad (III)$$

because $C_o \gg C_o'$ and $C_o \approx C_i$.

Materials and Methods

Solutions of the analytically pure compounds were made

in hexane, boiling at $63° - 68°C$, with concentrations (C_i)

ranging from 10 to 5000 µg per ml. Samples of 10 ml of the

hexane solution were shaken in pear-shaped separation funnels

with 40 ml demineralized water for one minute. After waiting

15 - 30 minutes the water layer was carefully separated and

the first few milliliters discarded. Of this water 20 ml was

again extracted with fresh hexane. The concentration (C_o') of

the insecticide in this layer was determined by gas-chromato-
graphy without further treatment. The distribution ratio was
calculated from Formula III.

Results and Discussion

Table 1 shows the results of estimating K. Each figure
is calculated from five independent experiments in which C_i =
1000 μg per ml.

TABLE 1

K values for different insecticides with
initial concentration 1000 μg per ml hexane.

	$C_o' \pm \sigma$ (μg per ml)	K
Lindane	0.580 ± 0.039	1730
Aldrin	0.010 ± 0.003	100000
Dieldrin	0.028 ± 0.002	36000
Heptachlor	0.009 ± 0.001	111000
Heptachlor epoxide	0.025 ± 0.004	40000
DDT	0.011 ± 0.005	91000

Lindane has a relatively small value for K. This is in
good agreement with its rather high solubility in water (6.8
ppm) (1). Dieldrin and heptachlor epoxide have intermediate
values for K. Their reported solubility is 0.186 and 0.35 ppm
respectively (2). The highest values are found for aldrin,
heptachlor and DDT, which have also the lowest solubility in
water: 0.027, 0.056 (2) and 0.025 ppm (1). Similar values for
K were obtained with other values of C_i although there were

considerable variations. The separation of the hexane and the water layer after the first shaking was critical. Standing overnight before separation of the water layer and extracting that layer with hexane again gave K = about 600,000 for aldrin. Any residual hexane in the water would decrease the K value found so that values in Table 1 are probably minimum.

Nevertheless it is clear that even when dissolved in a good solvent, a small quantity of the insecticide will partition into the water. Thus in organisms or organic material it is easy to conceive that insecticides which have accumulated for instance in fats, may become redistributed through the water phase.

References

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