Qualitative understanding of partition preferences

- Introduction
- Cavity model
- Rules for partitioning
- The cavity model in quantitative terms

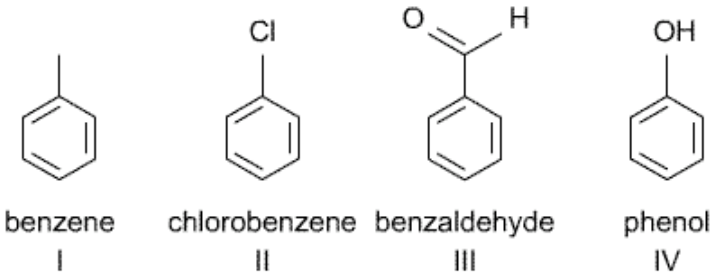
- Selftest
  - 1) What does the cavity model say?
    - Answer
  - 2) Main interactions ... ?
    - Answer
  - 3) Size of a *solute* molecule ... ?
    - Answer
  - 4) Size of the *solvent* molecule ... ?
    - Answer
  - 5) Interpretation of data
    - Answer
  - 6) "Like dissolves like"
    - Answer
  - 7) Concept maps
  - 8) Functional groups
    - Answer
  - 9) Illustration by given data?
    - Answer
  - 10) Evaluation of the software PcKocWIN
  - 11) H-bonds between given substances?
  - 12) Tendency to distribute
    - **Answer**
  - 13) Gas chromatography
    - Answer
  - 14) Henry's Law constant
    - Answer
  - 15) Quiz
- Problems
- Intermolecular interactions in every day life
- FAQ

12) Tendency to distribute

Question:

Rank the four compounds (I – IV) indicated below in the order of increasing tendency to distribute from (a) air into hexadecane (mimicking an apolar environment), (b) from air to olive oil, and (c) from air to water.

These are the respective volumina for the compounds:
benzene 0.716
chlorobenzene 0.839
benzaldehyde 0.873
phenol 0.775



Answer:

The order of experimental data does not always match the results of qualitative estimates. However, differences in K-values are usually smaller than a factor 3. You cannot expect a qualitative estimation to perform better than that. In addition, please note that a qualitative estimation cannot always be carried out.

air –> hexadecane

	benzene I	chlorobenzene II	benzaldehyde III	phenol IV
$K_{air/C_{16}H_{34}}$	1.6×10^{-3}	2.2×10^{-4}	1.0×10^{-4}	1.7×10^{-4}

The large difference between the partitioning coefficients of benzene and phenol are somewhat unexpected since they have a similar molecular size.

air –> olive oil

	benzene I	chlorobenzene II	benzaldehyde III	phenol IV
$K_{air/olive\ oil}$	1.5×10^{-3}	1.8×10^{-4}	n.a.	2.3×10^{-5}

air –> water

	benzene I	chlorobenzene II	benzaldehyde III	phenol IV
$K_{air/olive\ oil}$	0.23	0.15	1.1×10^{-3}	1.4×10^{-5}