

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

9) Which of the above rules can be illustrated by the given data?

Question:

Which of the [partitioning rules](#) can be illustrated by the partition data given below?

Hint: first classify all compounds according to the scheme (page "Polarity" or Table 3 in the textbook) as apolar, monopolar (H-donor or acceptor) and bipolar!

Compound / solvent combination	K _{solvent/air}	Example for partitioning rule ...					
		I only vdW-interactions occur:			II also H-bond interactions occur:		
		Rule 1 Case Ia apolar molecules in apolar or monopolar phases	Rule 2 Case Ib monopolar molecules in monopolar phases of the same polarity and in apolar phases	Rule 3 Case Ic bipolar molecules in apolar phases	Rule 4 Case IIa apolar molecule in bipolar phases	Rule 5 Case IIb >various chemicals in monopolar phases	Rule 6 other cases
ethanol / decane	38			✓			
ethanol / CCl ₄	115			✓			
ethanol / cyclohexane	45			✓			
butanone / cyclohexane	1301		✓				
butanone / butylether	533		✓				
butanone / CH ₂ Cl ₂	7272		✓				
dioxane / CCl ₄	4326		✓				
dioxane / cyclohexane	1106		✓				
dioxane / ethyl ether	2436		✓				

dioxane / chloroform	27366					✓	
dioxane / CH ₂ Cl ₂	18712					✓	
		Rule 1 Case Ia apolar molecules in apolar or monopolar phases	Rule 2 Case Ib monopolar molecules in monopolar phases of the same polarity and in apolar phases	Rule 3 Case Ic bipolar molecules in apolar phases	Rule 4 Case IIa apolar molecule in bipolar phases	Rule 5 Case IIb various chemicals in monopolar phases	Rule 6 other cases
toluene / CCl ₄	6621		✓				
toluene / decane	2638		✓				
toluene /cyclohexane	3831		✓				
dioxane / decane	813		✓				
dioxane / CCl ₄	4326		✓				
dioxane /cyclohexane	1106		✓				
dioxane / toluene	4080		✓				
dioxane /diethyl ether	2436		✓				
dioxane / benzylether	3122		✓				
butanone / decane	254		✓				
butanone / cyclohexane	1301		✓				
butanone / butylether	533		✓				
butanone / benzylether	985		✓				
		Rule 1 Case Ia apolar molecules in	Rule 2 Case Ib monopolar molecules in	Rule 3 Case Ic bipolar molecules in	Rule 4 Case IIa apolar molecule in	Rule 5 Case IIb various chemicals in	Rule 6 other cases

		apolar or monopolar phases	monopolar phases of the same polarity and in apolar phases	apolar phases	bipolar phases	monopolar phases	
water / heptane	4.47			✓			
water / 1,2,4-trichlorobenzene	12.5			✓			
water / tetrachloroethylene	6.67			✓			
ethanol / decane	38			✓			
ethanol / cyclohexane	45			✓			
ethanol / benzene	229						✓
ethanol / isopropylether	470						✓
ethanol / dioxane	1922						✓
toluene / butyl ether	3780		✓				
toluene / heptane	2928		✓				
toluene / chloroform	11890					✓	
octane / decane	6688	✓					
octane / CCl ₄	11142	✓					
octane /cyclohexane	11227	✓					
octane / toluene	7387	✓					
octane / ethyl ether	8287	✓					



proceed to answer

