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Partition Coefficient in n-Octanol and Water

Experiment 11 - Practical Notes

Name: _____ Roll no.: _____ Date: _____

Aim

To calculate the phase concentration ratio for a drug in n-octanol and water.

Principle

For a neutral species at equilibrium, P = Corganic/Cwater. If ionisation contributes at a stated pH, the ratio of total analytical concentrations is a distribution ratio D(pH). Temperature, pH and phase composition must be controlled.

Requirements

- Assigned neutral teaching solute and staff-approved shake-flask setup, or supplied equilibrium data.
- Matched phase-assay standards, recorded phase volumes, temperature and aqueous pH.

Procedure

1. Condition phases

For the bench method approved by the laboratory, mutually pre-saturate the phases and record actual phase volumes. For a supplied-data exercise, read these conditions from the staff record.

2. Establish equilibrium

Use the staff-approved controlled mixing and settling method with the assigned solute loading. Avoid persistent emulsion and container adsorption.

3. Identify layers

Verify layer identity from the prescribed check; do not rely only on an assumed solvent order.

4. Measure both phases

Determine concentrations using phase-appropriate calibration and dilution factors. Do not substitute raw absorbance ratios from different solvent matrices.

5. Check mass balance

Calculate Corganic Vorg + Cwater Vwater and compare with initial solute mass. Investigate unexplained loss before accepting the ratio.

6. Report

Calculate P or D as applicable and $\log_{10}$ of that ratio. State phase volumes, temperature, pH, ionisation assumption and replicate agreement.

Observations and Record

Record	Entry
Organic / aqueous phase volumes	_____
Concentrations after dilution correction	_____
Initial / recovered total solute mass	_____
P or D(pH) / $\log_{10}$ value	_____

Worked Example

The numbers below are illustrative; enter your own observations in the record.

- For C_o = 4.00 mg/mL and Cw = 0.500 mg/mL, P = 8.00 and $\log_{10}$ P = 0.9031.
- At 10.0 mL in each phase, recovered mass = 4.00×10.0 + 0.500×10.0 = 45.0 mg. Compare with an assigned initial 45.0 mg.

Result

Record the observed outcome and calculated value, with units. State whether the stated laboratory specification was met; do not copy the worked example as your result.

Precautions

- Use the instructor's assigned material and apparatus; record actual temperature and units with every measured property.
- Check instrument calibration and use repeat readings rather than a single convenient result.
- Compare a marketed teaching formulation only under the same method and conditions; its excipients can change the property.

Viva Questions and Answers

1. Why measure both phases?

It supports both the ratio and a mass-balance check.

2. When should the result be called D?

When the ratio concerns total species at a stated pH and ionisation affects distribution.

3. Is the ratio obtained in one solvent transferable to another?

No. The solvent system defines the partition behaviour.

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