# SNS COLLEGE OF PHARMACY AND HEALTH SCIENCES

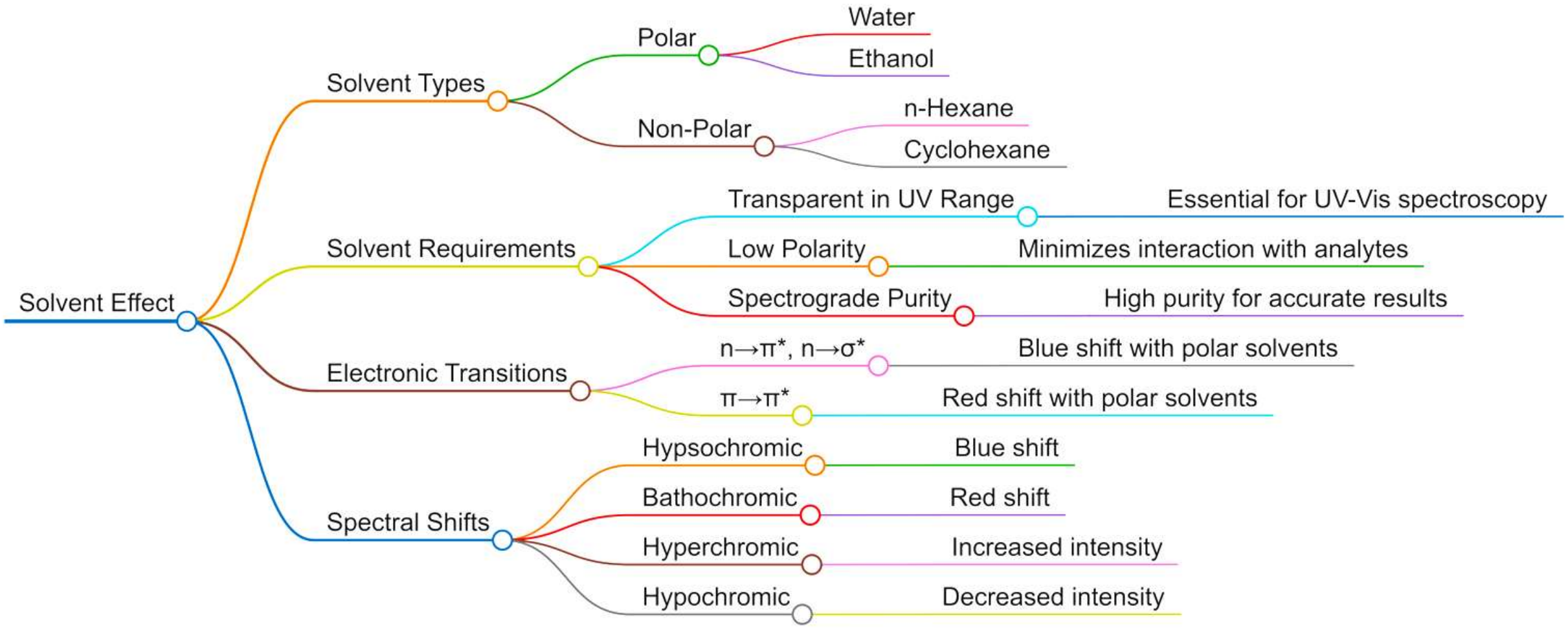
*Affiliated To The Tamil Nadu Dr. MGR Medical University, Chennai*
*Approved by Pharmacy Council of India, New Delhi.*
**Coimbatore -641035**

## COURSE NAME: INSTRUMENTAL METHODS OF ANALYSIS (BP 701 T)

## VII SEM/ IV YEAR

## TOPIC 3: Solvent effect on absorption spectra

# MINDMAP

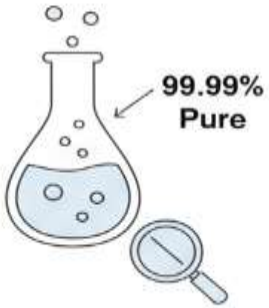

Solvent Effect
Solvent Types
Polar
Water
Ethanol
Non-Polar
n-Hexane
Cyclohexane
Solvent Requirements
Transparent in UV Range
Essential for UV-Vis spectroscopy
Low Polarity
Minimizes interaction with analytes
Spectrograde Purity
High purity for accurate results
Electronic Transitions
n→π*, n→σ*
Blue shift with polar solvents
π→π*
Red shift with polar solvents
Spectral Shifts
Hypsochromic
Blue shift
Bathochromic
Red shift
Hyperchromic
Increased intensity
Hypochromic
Decreased intensity

# What is solvent?

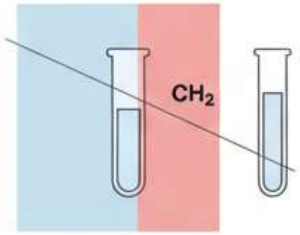
A liquid that dissolves a solute to form a solution at a specified temperature.

## Requirements for UV solvents:

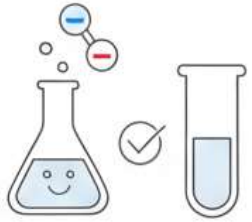
**1. High Purity (Spectrograde)**



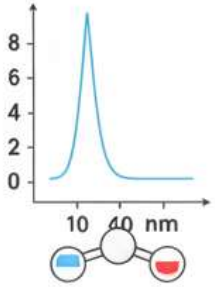

**2. UV Transparency**




**3. Non-Reactive**

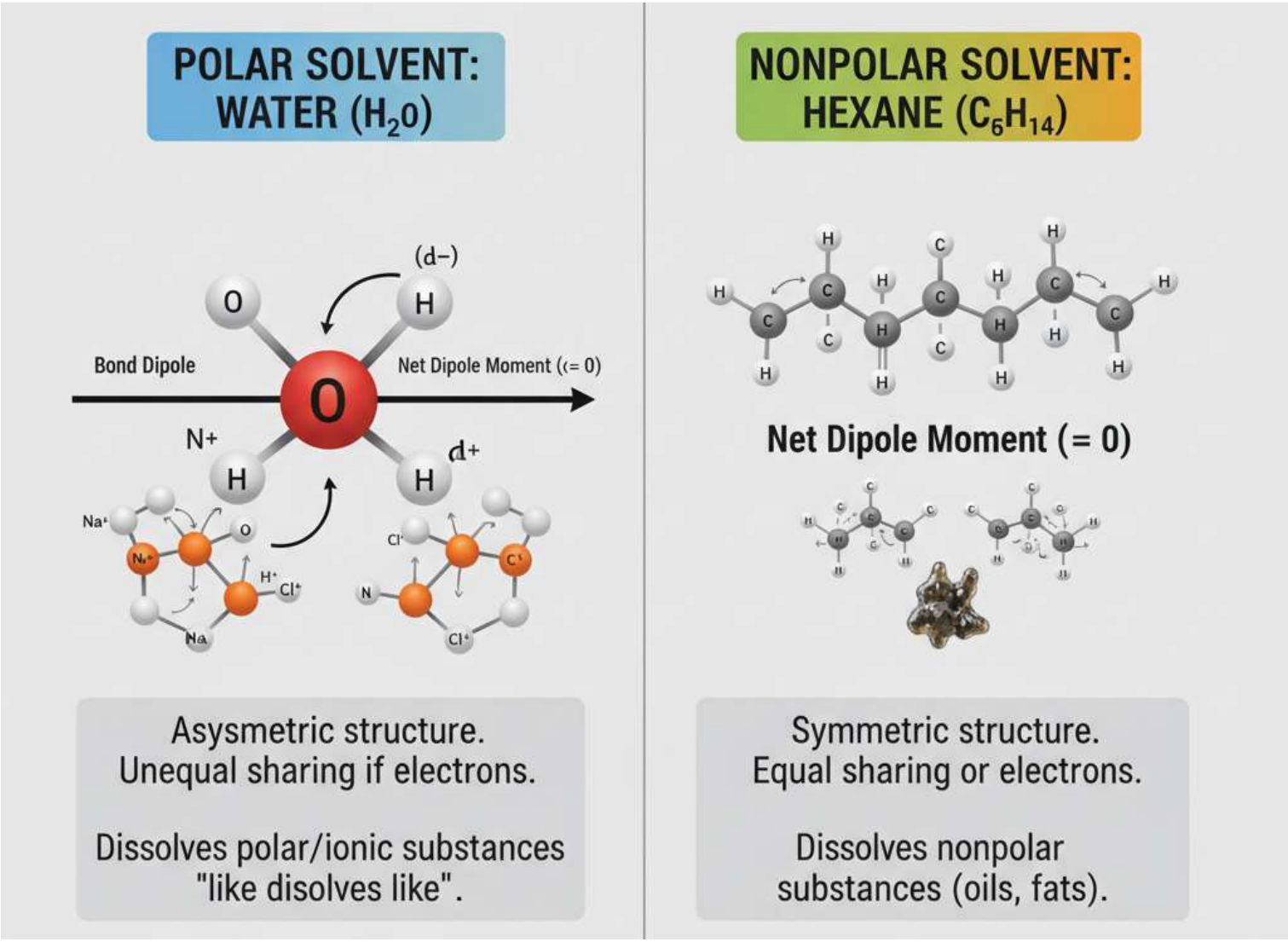


**4. Low Dipole Moment**



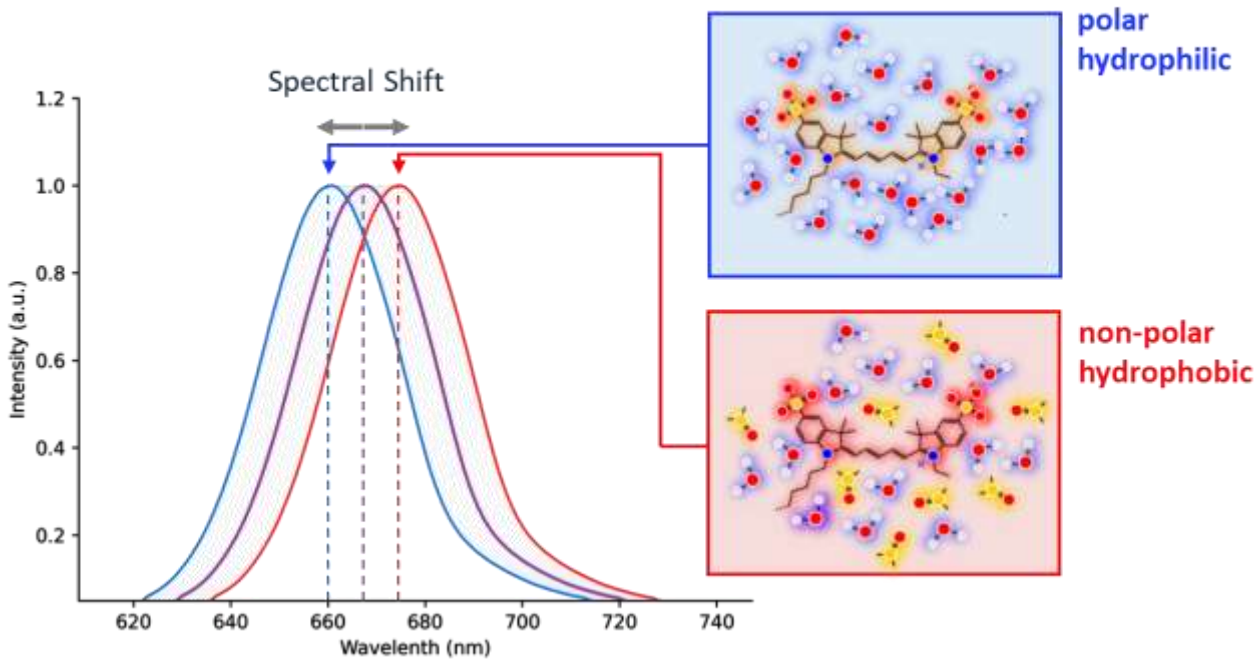

Non-Polar Solvent

# Classification of solvents based on polarity:

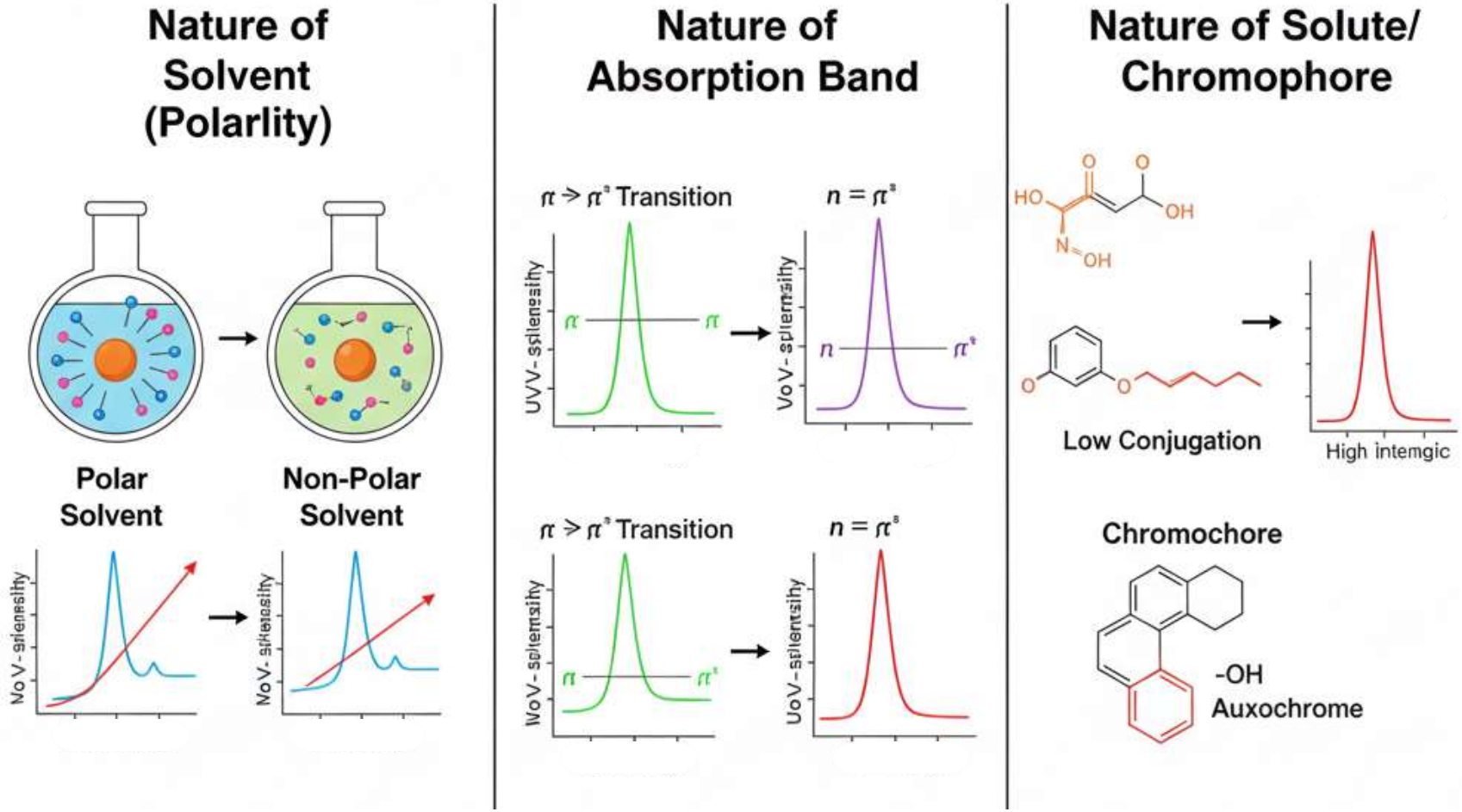


# Solvent effect

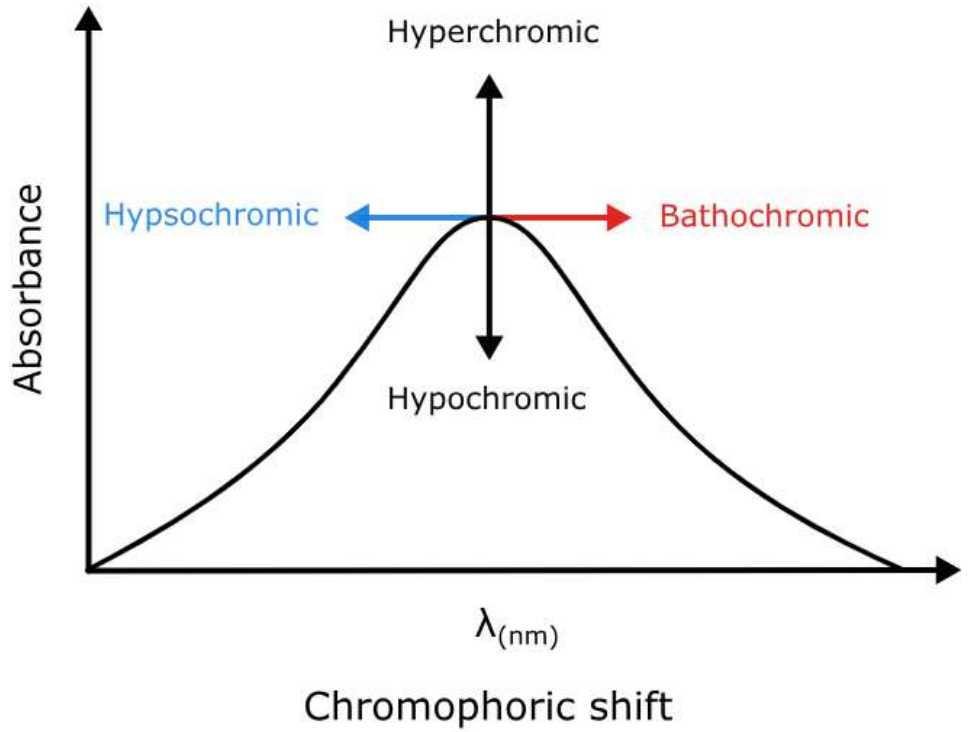
**Unexpected shifts in λmax due to solvent choice.**



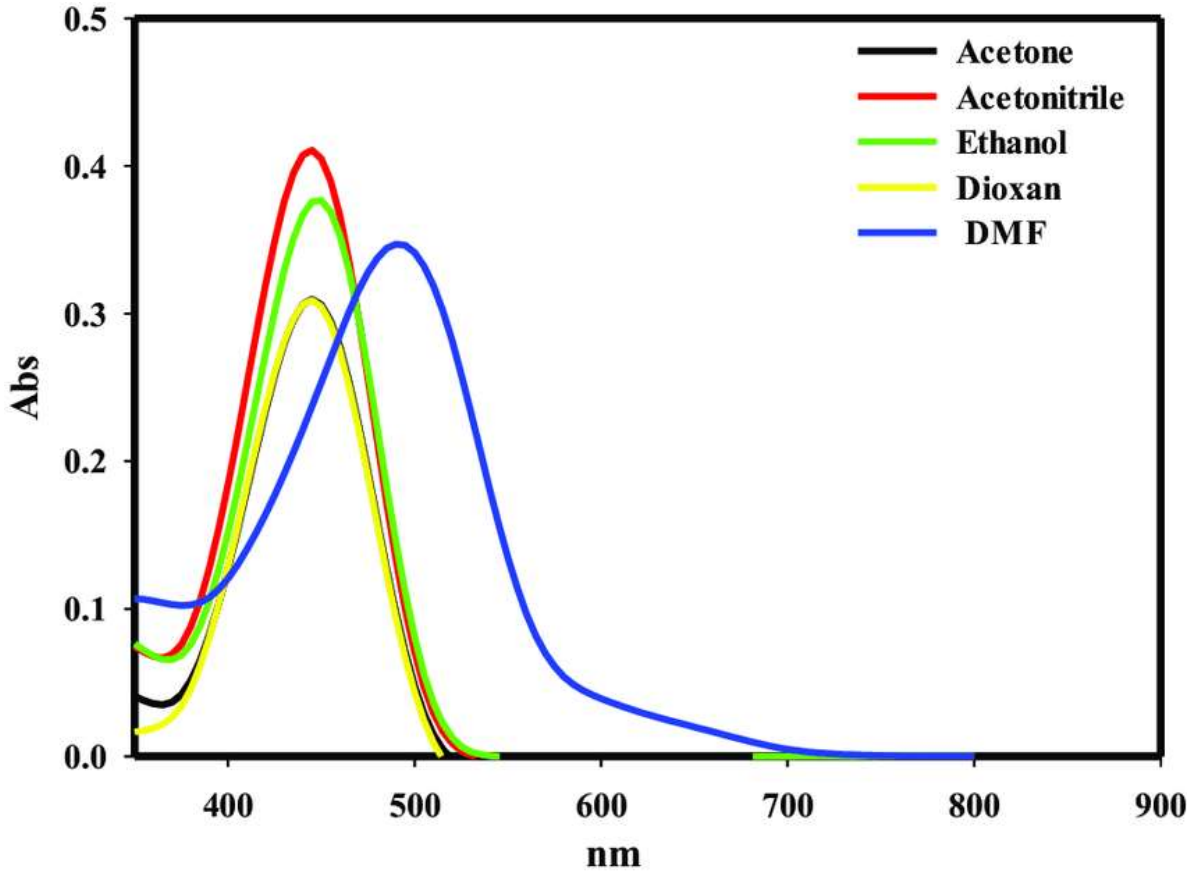
# Key factors influencing the problem



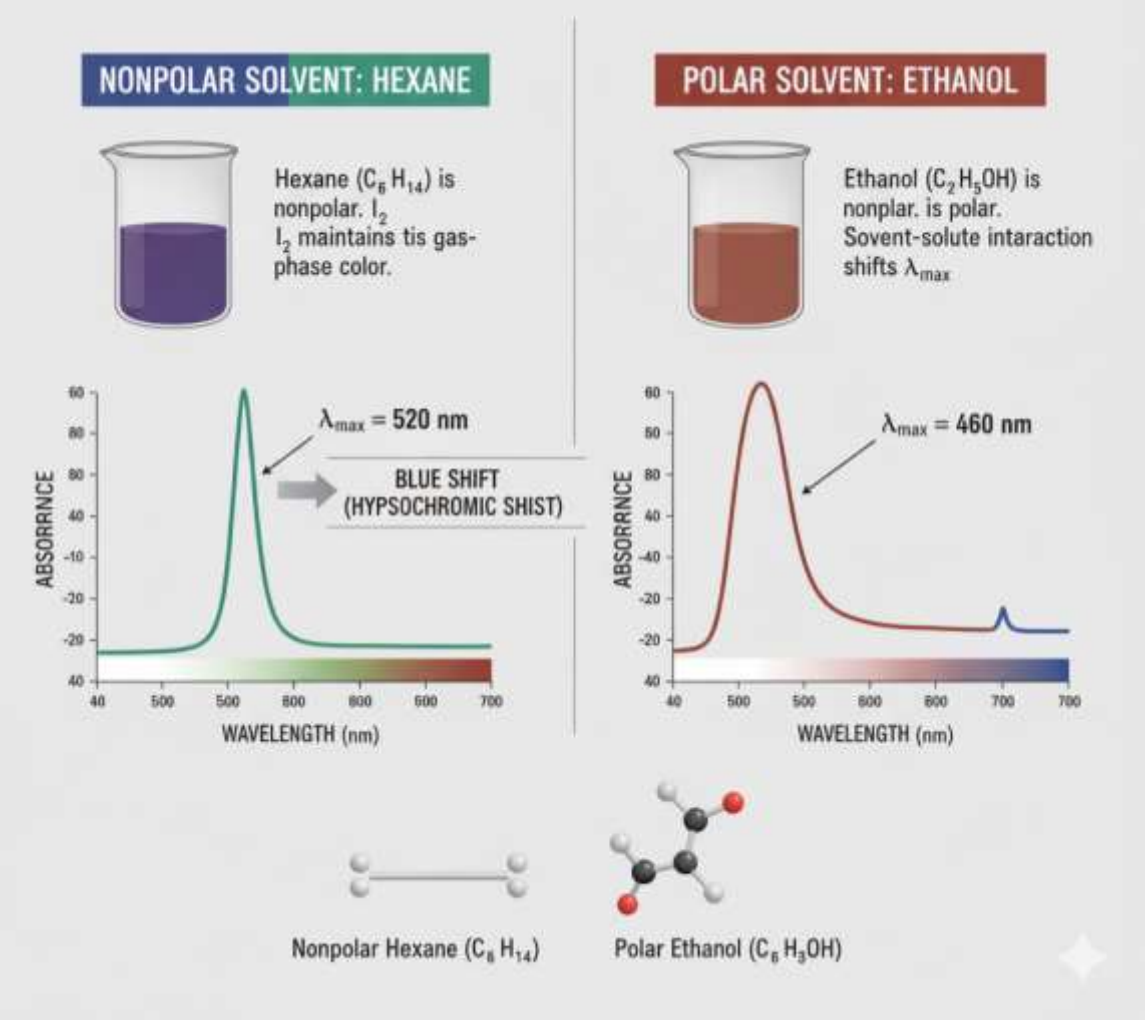
# Solvent effects can cause spectral shifts



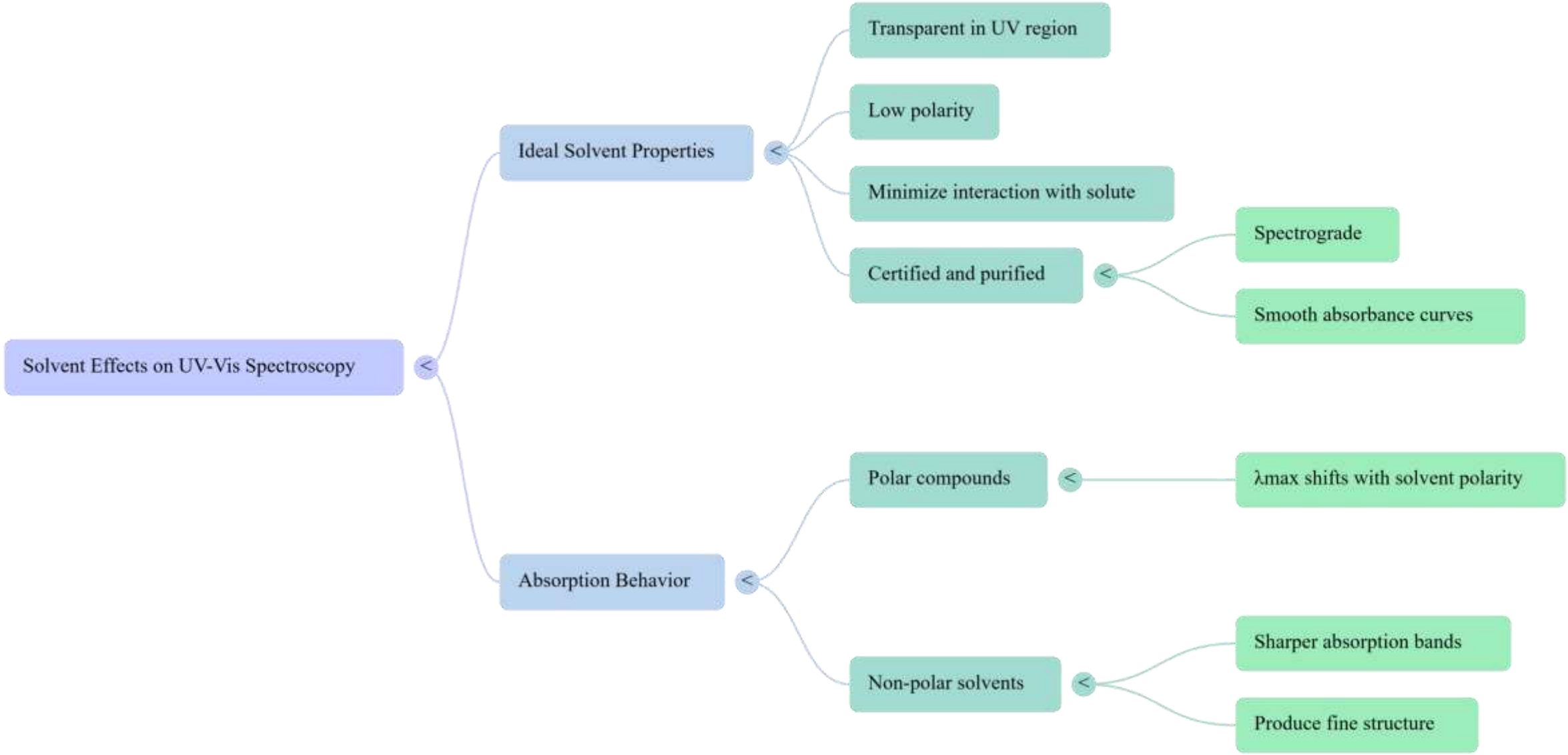
# Solvent Effects on λmax



# Solvent Effects on λmax: Example

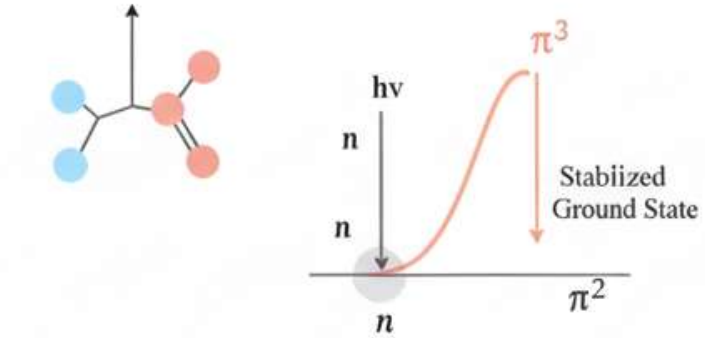


# Requirements for UV Spectroscopy Solvents

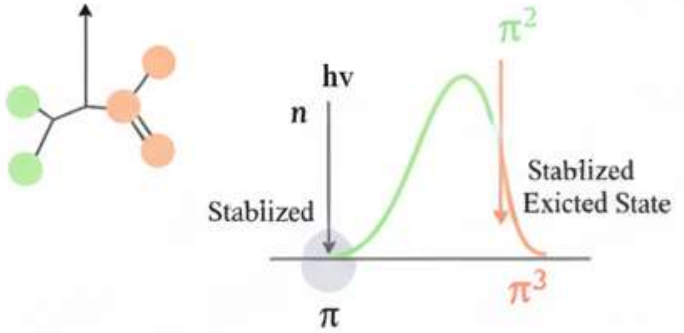


# Solvent Polarity and Electronic Transitions

## $n-\pi^*$ and $n-so^*$ Transitions



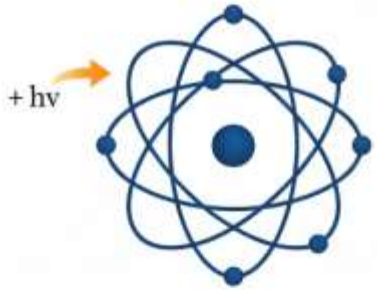

## $\pi-\pi^*$ $\pi-\pi^*$ Transitions:



# Solvent Stabilization Mechanisms

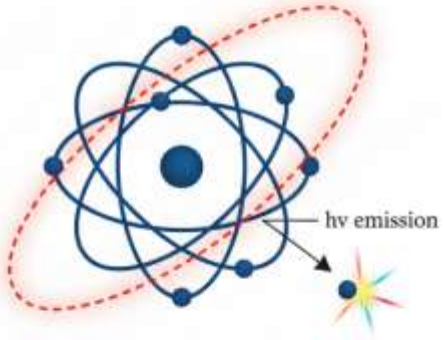
## Ground vs. Excited State

### GROUND STATE

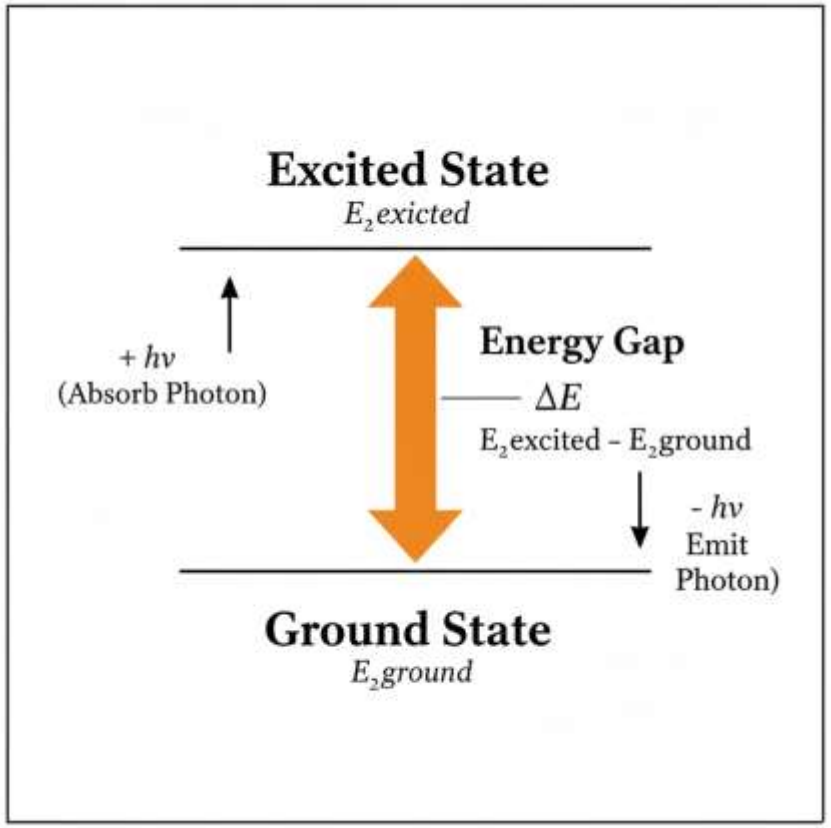



- Lowest Energy
- Stable Orbitals
- Electrons Close to Nucleus

### EXCITED STATE




- Higher Energy
- Unstable Orbitals
- Electron Jumps Farther
- Emits Light (Photon)



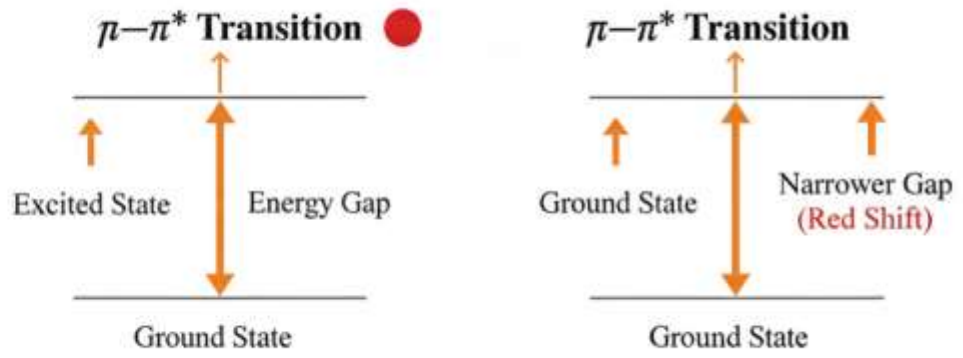
# Solvent Stabilization Mechanisms

## Energy Gap Changes

### Solvent Polarity Effects on Electronic Transitions

➢ Increased solvent polarity widens energy gap for $n \rightarrow \pi^*$ (blue shift).

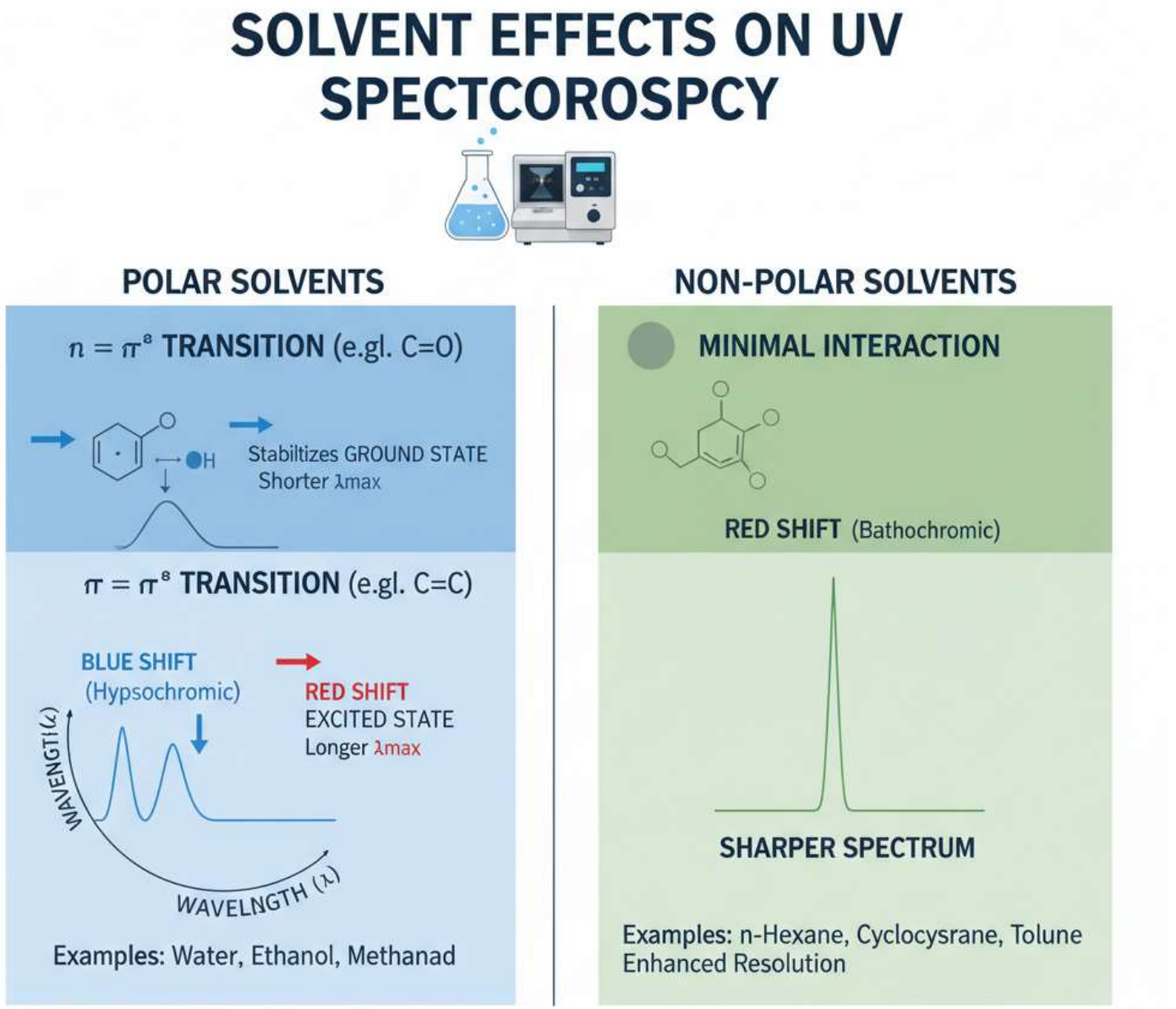

➢ Decreased energy gap for $\pi \rightarrow \pi^*$ (blue shift).



# Common Solvents and their λmax

| Solvent | λmax (nm) | | |
|---|---|---|---|
| Water | 191 | 191nm | 191 |
| Methanal | 215 | 10nm | 203 |
| Ethanol | 204 | 25nm | 277 |
| Choroform Carbon Tetttorcllade | 237 | 30nm | |
| Benzene | 260 | 37nm | |
| Benzene | 260 | 58nm | |
| Tethalharvofuran | 220 | 20nm | |

# Summary

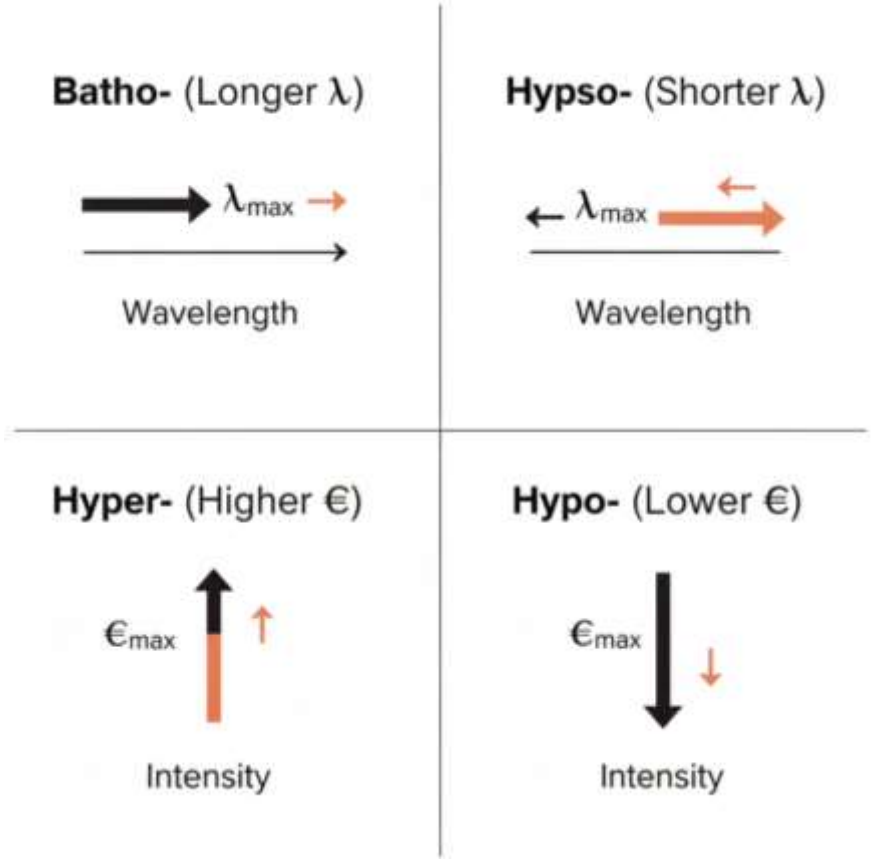

SOLVENT EFFECTS ON UV SPECTCOROSPCY
POLAR SOLVENTS
n = π* TRANSITION (e.gl. C=O)
Stabiltizes GROUND STATE
Shorter λmax
π = π* TRANSITION (e.gl. C=C)
BLUE SHIFT
(Hypsochromic)
RED SHIFT
EXCITED STATE
Longer λmax
WAVENGTI(λ)
WAVELNGTH (λ)
Examples: Water, Ethanol, Methanad
NON-POLAR SOLVENTS
MINIMAL INTERACTION
RED SHIFT (Bathochromic)
SHARPER SPECTRUM
Examples: n-Hexane, Cyclocysrane, Tolune
Enhanced Resolution

# Assessment: MCQ

1. **What is the effect of a polar solvent on a π→π* transition?**

# Assessment: MCQ

**1. What is the effect of a polar solvent on a π→π* transition?**

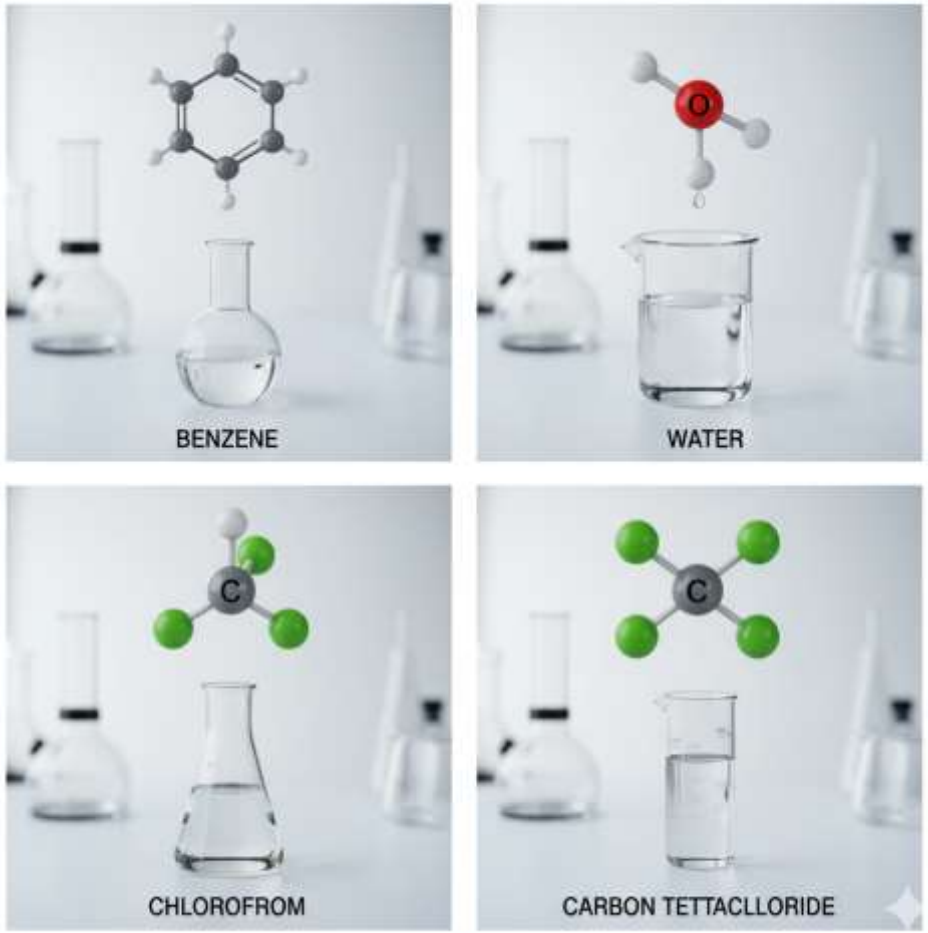


# Assessment: MCQ

2. **Which solvent is suitable for UV spectroscopy due to its transparency below 200 nm?**

# Assessment: MCQ

2. **Which solvent is suitable for UV spectroscopy due to its transparency below 200 nm?**



# Assessment: MCQ

**3. What is meant by solvatochromism?**

# Assessment: MCQ

**3. What is meant by solvatochromism?**

**A) Change in color due to pH**

**B) Fluorescence quenching by solvent**


**C) Change in absorption due to solvent polarity**

**D) Temperature-dependent absorption**

# References


1. Skoog DA, Holler FJ, Crouch SR. *Principles of Instrumental Analysis*. 7th ed. Boston (MA): Cengage Learning; 2018. Chapter 13, Molecular UV-Visible Spectroscopy.
2. Willard HH, Merritt LL, Dean JA, Settle FA. *Instrumental Methods of Analysis*. 7th ed. Belmont (CA): Wadsworth Publishing; 1988. Chapter 6, Spectrometric Methods.
3. Silverstein RM, Webster FX, Kiemle DJ. *Spectrometric Identification of Organic Compounds*. 8th ed. Hoboken (NJ): John Wiley & Sons; 2014. Chapter 8, Ultraviolet Spectroscopy.
4. Kemp W. *Organic Spectroscopy*. 3rd ed. Basingstoke (UK): Macmillan; 1991. Chapter 1, Ultraviolet and Visible Spectroscopy.
5. Sharma YR. *Elementary Organic Spectroscopy: Principles and Chemical Applications*. 5th ed. New Delhi: S Chand Publishing; 2013. Chapter 1, Ultraviolet Spectroscopy.


Thank you!