

Advanced UV/Visible Spectroscopy MCQs

Application of Ultraviolet/Visible Molecular Absorption Spectrometry

20 Multiple-Choice Questions - 15 non-calculation questions and 5 theoretical wavelength calculations with molecular structures

Circle the single best answer. The answer key and calculation checks are provided at the end of the file.

Part I: Non-Calculation Questions

1. A carbonyl-containing compound exhibits two absorption bands: one at approximately 190 nm with $\epsilon \approx 9,000$, and another at approximately 285 nm with $\epsilon \approx 20$. Which assignment is most appropriate?

- A. The 190 nm band is $n \rightarrow \pi^*$ while the 285 nm band is $\pi \rightarrow \pi^*$.
- B. Both bands arise from $n \rightarrow \sigma^*$ transitions.
- C. The 190 nm band is $\pi \rightarrow \pi^*$ while the 285 nm band is $n \rightarrow \pi^*$.
- D. The 190 nm band is $\sigma \rightarrow \sigma^*$ while the 285 nm band is $n \rightarrow \sigma^*$.

2. Which sequence correctly arranges the following transitions from the highest energy requirement to the lowest energy requirement?

- A. $n \rightarrow \pi^* > \pi \rightarrow \pi^* > n \rightarrow \sigma^* > \sigma \rightarrow \sigma^*$
- B. $\sigma \rightarrow \sigma^* > n \rightarrow \sigma^* > \pi \rightarrow \pi^* > n \rightarrow \pi^*$
- C. $\pi \rightarrow \pi^* > \sigma \rightarrow \sigma^* > n \rightarrow \pi^* > n \rightarrow \sigma^*$
- D. $n \rightarrow \sigma^* > \sigma \rightarrow \sigma^* > n \rightarrow \pi^* > \pi \rightarrow \pi^*$

3. An absorption band has a molar absorptivity of $650 \text{ L mol}^{-1} \text{ cm}^{-1}$. According to the chapter, which interpretation is most appropriate?

- A. It represents a highly allowed transition with a probability close to unity.
- B. It is classified as a low-intensity band and is probably associated with a forbidden transition.
- C. It must arise exclusively from a $\sigma \rightarrow \sigma^*$ transition.
- D. It cannot be detected using UV/Visible spectrometry.

4. Which molecular change most directly produces a bathochromic shift in the absorption of a conjugated chromophore?

- A. Increasing the energy difference between the HOMO and LUMO.
- B. Interrupting conjugation with an sp^3 -hybridized carbon.
- C. Lowering the energy of the π^* orbital through greater electron delocalization.
- D. Removing all alkyl substituents without changing the conjugated system.

5. A saturated compound containing a halogen atom absorbs weakly at approximately 173 nm. Which transition is most likely responsible?

- A. $n \rightarrow \sigma^*$
- B. $n \rightarrow \pi^*$
- C. $\pi \rightarrow \pi^*$
- D. Charge-transfer transition

6. Which statement concerning the orbitals of a carbon-carbon double bond is correct?

- A. It consists of two π molecular orbitals formed by head-on overlap.
- B. It contains one σ orbital and one π orbital, with the π orbital formed by parallel overlap of atomic p orbitals.
- C. It contains only a σ orbital because π orbitals are nonbonding.
- D. It contains one bonding orbital and no corresponding antibonding orbitals.

7. Why can normal n-alkanes commonly be used as solvents for measurements in the ordinary UV/Visible region?

- A. Their $n \rightarrow \pi^*$ transitions occur exclusively in the visible region.
- B. They contain highly conjugated chromophores with very low absorptivity.
- C. Their principal $\sigma \rightarrow \sigma^*$ absorption occurs mainly below approximately 185 nm.
- D. Their absorption bands are eliminated by hydrogen bonding.

8. Which description best distinguishes an auxochrome from a chromophore?

- A. An auxochrome is always a conjugated carbonyl group.
- B. An auxochrome generally contains unshared electron pairs and may shift the absorption of an attached chromophore to a longer wavelength.
- C. An auxochrome absorbs only through $\sigma \rightarrow \sigma^*$ transitions.
- D. An auxochrome decreases wavelength by increasing the HOMO-LUMO energy gap.

9. A molecule containing both n and π electrons displays two separate bands in hexane. When the solvent is changed to ethanol, the bands move closer together. Which combination best explains this observation?

- A. The $\pi \rightarrow \pi^*$ band undergoes a blue shift, while the $n \rightarrow \pi^*$ band undergoes a red shift.
- B. Both bands undergo identical bathochromic shifts.
- C. The $\pi \rightarrow \pi^*$ band undergoes a red shift, while the $n \rightarrow \pi^*$ band undergoes a blue shift.
- D. The $\pi \rightarrow \pi^*$ band becomes forbidden, while the $n \rightarrow \pi^*$ band disappears.

10. Ethylene exhibits a strong $\pi \rightarrow \pi^*$ absorption, whereas acetone exhibits a weak $n \rightarrow \pi^*$ absorption at a longer wavelength. Which statement is correct?

- A. The acetone transition requires more energy and has a greater transition probability.
- B. The ethylene transition requires less energy because it occurs at a shorter wavelength.
- C. The acetone transition requires less energy but has a much lower transition probability.
- D. Both transitions have approximately equal molar absorptivities.

11. For a carbonyl compound possessing nonbonding electrons, which pair most reasonably represents the orbitals involved in its lowest-energy electronic transition?

- A. HOMO = σ , LUMO = σ^*
- B. HOMO = π , LUMO = σ^*
- C. HOMO = n , LUMO = π^*
- D. HOMO = π^* , LUMO = σ^*

12. Which assignment of electromagnetic spectral regions is correct?

- A. 250 nm: visible; 500 nm: near infrared; 900 nm: microwave.
- B. 250 nm: near ultraviolet; 500 nm: visible; 900 nm: near infrared.
- C. 250 nm: far infrared; 500 nm: near ultraviolet; 900 nm: visible.
- D. 250 nm: microwave; 500 nm: visible; 900 nm: far ultraviolet.

13. Compared with an isolated or unconjugated diene, a conjugated diene normally absorbs at a longer wavelength primarily because:

- A. Conjugation raises the π^* energy level and increases antibonding character.
- B. Delocalization lowers the π^* energy level and decreases the energy required for excitation.
- C. Conjugation converts all π electrons into nonbonding electrons.
- D. The $\sigma \rightarrow \sigma^*$ transition becomes the lowest-energy transition.

14. An absorption spectrum shows a reduction in the height of a band, while the position of $\lambda_{\max}$ remains essentially unchanged. This effect is called:

- A. Bathochromism
- B. Hypsochromism
- C. Hyperchromism
- D. Hypochromism

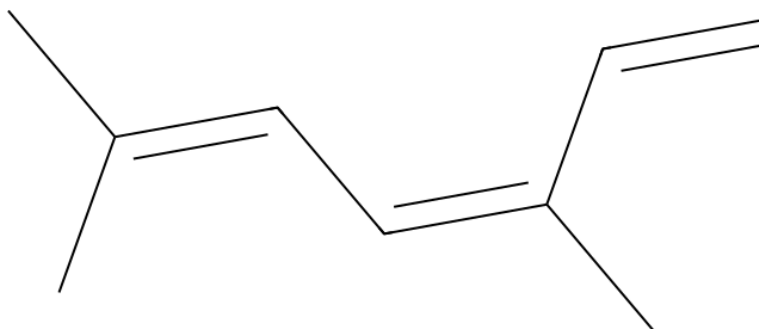
15. According to the practical conditions stated in the chapter, which absorption band is the most suitable for analysis using an ordinary UV/Visible instrument?

- A. $\lambda_{\max} = 175 \text{ nm}$, $\epsilon = 8,000$
- B. $\lambda_{\max} = 205 \text{ nm}$, $\epsilon = 700$
- C. $\lambda_{\max} = 192 \text{ nm}$, $\epsilon = 1,500$
- D. $\lambda_{\max} = 180 \text{ nm}$, $\epsilon = 500$

Part II: Theoretical $\lambda_{\max}$ Calculations

Use the Woodward-Fieser rules provided at the end of the chapter.

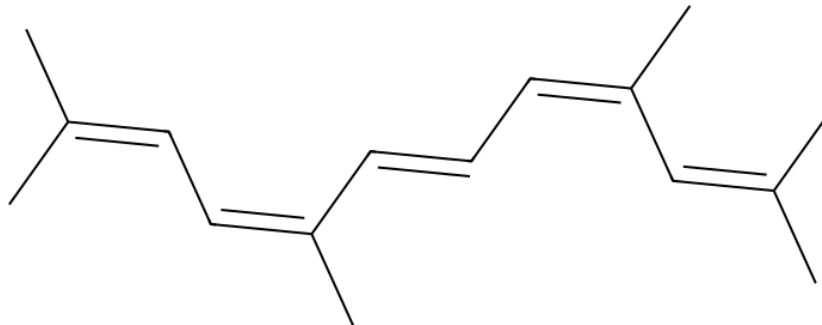
16. Calculate the theoretical $\lambda_{\max}$ for the following acyclic conjugated triene.



Q16: Acyclic conjugated triene

- A. 247 nm
- B. 257 nm
- C. 262 nm
- D. 272 nm

17. The following compound contains five conjugated double bonds. Using the equation given for systems containing more than four conjugated double bonds, calculate its theoretical $\lambda_{\max}$.

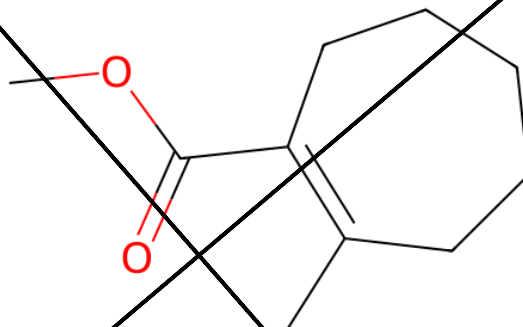


Q17: Conjugated pentaene

- A. 332 nm
- B. 342 nm
- C. 352 nm
- D. 362 nm

20. Calculate the theoretical λ_{max} of the following conjugated ester in water. Include the correction for an endocyclic double bond in a seven-membered ring and the solvent correction.

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Q20: Conjugated ester in a seven-membered ring

- A. 222 nm
- B. 234 nm
- C. 242 nm
- D. 250 nm

Model Answer Key

1	C	6	B	11	C	16	C
2	B	7	C	12	B	17	B
3	B	8	B	13	B	18	B
4	C	9	C	14	D	19	D
5	A	10	C	15	C	20	C

Calculation Check

Question 16

$$\lambda_{\max} = 217 + 30 + 3(5) = 262 \text{ nm.}$$

Question 17

For five conjugated double bonds and six alkyl substituents:

$$\lambda_{\max} = 114 + 6(5) + 5[48 - 1.7(5)] = 341.5 \approx 342 \text{ nm.}$$

Question 18

$$\lambda_{\max} = 215 + 30 + 10 + 12 + 2(18) = 303 \text{ nm.}$$

Question 19

$$\lambda_{\max} = 202 + 10 + 2(12) + 5 = 241 \text{ nm.}$$

Question 20

$$\lambda_{\max} = 195 + 10 + 2(12) + 5 + 8 = 242 \text{ nm.}$$