Advanced IR Spectrometry MCQs

Chapter 16 - An Introduction to Infrared Spectrometry

15 Very Difficult Multiple-Choice Questions

Each question includes four options arranged clearly beneath it. The complete model answer key is provided at the end of the document.

Prepared from: IA (-6-) Lecture IR-1

Questions

Question 1

Which statement most accurately describes the relative molecular energy spacings and the radiation commonly associated with them?

A. $\Delta E_{rot} >> \Delta E_{vib} >> \Delta E_{el}$, with vibrational transitions mainly in the microwave region.

B. $\Delta E_{el} >> \Delta E_{vib} >> \Delta E_{rot}$, with vibrational transitions mainly associated with infrared radiation.

C. $\Delta E_{vib} >> \Delta E_{el} >> \Delta E_{rot}$, with electronic transitions requiring lower energy than vibrations.

D. $\Delta E_{el} \approx \Delta E_{vib} >> \Delta E_{rot}$, because electronic and vibrational transitions occur over essentially the same spectral range.

Question 2

An IR spectrum is recorded in % transmittance mode. Which observation correctly indicates strong absorption by the sample?

A. An upward peak approaching 100% transmittance.

B. A downward band corresponding to a pronounced decrease in %T.

C. A horizontal region at 100%T because all incident radiation has been absorbed.

D. A peak whose position depends only on its intensity and not on wavenumber.

Question 3

CO_2 has a permanent molecular dipole moment of approximately zero, yet it absorbs IR radiation in selected vibrational modes. Which explanation is correct?

A. Any molecule containing polar bonds is automatically IR active in every vibrational mode.

B. CO_2 absorbs because IR radiation produces electronic transitions that generate a permanent dipole.

C. A vibration is IR active when it produces a net change in molecular dipole moment and the incident radiation matches its natural vibrational frequency.

D. Only molecules with a permanent dipole moment before vibration can absorb infrared radiation.

Question 4

According to the sample-handling notes in the chapter, which procedure is most appropriate?

A. A liquid sample must first be mixed with powdered KBr and compressed into a disk.

B. A solid sample may be mixed with KBr and compressed into a disk, whereas a liquid may be examined directly without such a carrier preparation.

C. NaCl is always preferred to KBr because KBr absorbs more water and is mechanically harder.

D. Both solids and liquids must always be converted into KBr pellets before IR analysis.

Question 5

Which set correctly matches the three types of molecular transitions discussed for IR spectroscopy?

A. Rotational: most important qualitative mid-IR transition; vibrational: below 100 cm^{-1}; vibrational-rotational: electronic excitation plus rotation.

B. Rotational: low-energy transitions that may form sharp lines subdividing gas-phase vibrational peaks; vibrational-rotational: simultaneous contribution from bond vibration and molecular rotation; vibrational: most important for qualitative mid-IR analysis.

C. Rotational: occurs only in symmetric molecules; vibrational-rotational: independent of dipole moment; vibrational: restricted to the microwave region.

D. Rotational: requires electronic excitation; vibrational-rotational: occurs only in solids; vibrational: always produces a single absorption band.

Question 6

Consider the following statements about molecular vibrations:

I. Asymmetric stretching generally occurs at a higher wavenumber than symmetric stretching.
II. Stretching generally occurs at a higher wavenumber than bending.
III. Scissoring and rocking are in-plane bending modes.
IV. Wagging and twisting are out-of-plane bending modes.

Which option is correct?

A. I and II only

B. II, III, and IV only

C. I, II, III, and IV

D. I and IV only

Question 7

Which assignment is most consistent with the IR regions emphasized in the chapter?

A. 3350 cm^{-1} → triple-bond region; 2250 cm^{-1} → fingerprint region; 1700 cm^{-1} → X-H region

B. 3300 cm^{-1} → X-H region; 2250 cm^{-1} → triple-bond region; 1700 cm^{-1} → double-bond region; 1000 cm^{-1} → fingerprint region

C. 3300 cm^{-1} → fingerprint region; 2250 cm^{-1} → double-bond region; 1700 cm^{-1} → triple-bond region

D. 3300 cm^{-1} → double-bond region; 2250 cm^{-1} → X-H region; 1700 cm^{-1} → fingerprint region

Question 8

For two bonds involving the same pair of atoms, assume their force constants are approximately 5×10^2, 1×10^3, and 1.5×10^3 N/m for single, double, and triple bonds, respectively. Based on

$$\bar{\nu} \propto \sqrt{(k/\mu)}$$

which relationship between their approximate stretching wavenumbers is expected?

A. $\bar{\nu}_{single} > \bar{\nu}_{double} > \bar{\nu}_{triple}$

B. $\bar{\nu}_{triple} : \bar{\nu}_{double} : \bar{\nu}_{single} \approx \sqrt{3} : \sqrt{2} : 1$

C. $\bar{\nu}_{triple} : \bar{\nu}_{double} : \bar{\nu}_{single} = 3 : 2 : 1$ exactly

D. All three have equal wavenumbers because their reduced masses are identical.

Question 9

Which combination of theoretical vibrational-mode counts is correct?

A. $CS_2 = 3$, $H_2O = 4$, $CCl_4 = 9$

B. $CS_2 = 4$, $H_2O = 3$, $CCl_4 = 9$

C. $CS_2 = 4$, $H_2O = 3$, $CCl_4 = 6$

D. $CS_2 = 3$, $H_2O = 3$, $CCl_4 = 15$

Question 10

A molecule is calculated to possess 12 normal vibrational modes, but considerably fewer experimental IR peaks are detected. Which combination could explain this observation according to the chapter?

A. Some vibrations do not change the dipole moment; some vibrational energies are identical or nearly identical; some absorptions are too weak; and some vibrations lie outside the instrument range.

B. Every theoretical vibration necessarily produces one strong and completely resolved IR peak.

C. The missing peaks can only be explained by overtones.

D. Combination and difference bands always reduce the number of experimentally observed peaks.

Question 11

Suppose a fundamental vibration occurs at wavenumber $\bar{\nu}$. Which statement about additional bands is correct?

A. The fundamental transition corresponds to $V_0 \rightarrow V_2$, whereas the first overtone is $V_0 \rightarrow V_1$.

B. Overtones are normally stronger than fundamental bands and occur at approximately $\bar{\nu}/2$ and $\bar{\nu}/3$.

C. A combination band may occur at $\bar{\nu}_3 = \bar{\nu}_1 + \bar{\nu}_2$, whereas a difference band may occur at $\bar{\nu}_3 = \bar{\nu}_1 - \bar{\nu}_2$.

D. All mathematically possible combination and difference bands must necessarily appear experimentally.

Question 12

Which ordering best reflects the factors affecting the frequency of IR absorption discussed in the chapter?

A. Heavy atoms > light atoms; weak bonds > strong bonds; bending > stretching

B. Light reduced mass > heavy reduced mass; strong bond > weak bond; stretching > bending

C. Heavy reduced mass > light reduced mass; strong bond > weak bond; bending > stretching

D. Bond strength has no effect provided the atoms are unchanged.

Question 13

Two compounds contain absorptions at nearly the same C-H stretching frequency. Compound X contains many C-H bonds contributing at that frequency, while compound Y contains only a few. In addition, X contains a strongly polar C=O bond whereas Y contains a relatively nonpolar C=C bond. Which prediction is most consistent with the chapter?

A. Y should necessarily show larger absorptions because fewer bonds give sharper peaks.

B. The C=O absorption can be strong because of its large dipole change, and numerous C-H bonds absorbing at the same frequency can produce a larger band.

C. C=C must absorb more strongly than C=O because double bonds always have the largest dipole moment.

D. Band intensity depends entirely on force constant and is unrelated to the number of absorbing bonds or dipole strength.

Question 14

Which description of the CO_2 spectrum is correct?

A. CO_2 is nonlinear and possesses three vibrational modes, all giving separate IR bands.

B. CO_2 has four normal modes; its symmetric stretch is IR inactive, its asymmetric stretch gives an absorption near 2330 cm^{-1}, and its two equivalent bending modes have identical energy and appear as one band near 667 cm^{-1}.

C. CO_2 produces four experimentally separate peaks because each normal mode must give a unique IR absorption.

D. Its two bending vibrations occur at different energies because they are oriented 90° apart.

Question 15

Which option contains only correct statements about the IR sources described in the chapter?

A. The Nernst glower is a silicon carbide rod; the Globar is made of rare-earth oxides; and the mercury arc is mainly used in the near-IR region.

B. The Globar is a SiC rod heated to roughly 1300-1500 K; the incandescent nichrome source has lower intensity but longer life; and a high-pressure mercury arc is useful for the far-IR region above about 50 µm.

C. The tungsten filament lamp is mainly used from 900-1100 cm^{-1}, while the CO_2 laser is mainly used from 4000-12,800 cm^{-1}.

D. The CO_2 laser is a blackbody thermal source used exclusively in solid-state sample analysis.

Model Answers

Answer key for Questions 1-15

Q1	**B**	**Q6**	**C**	**Q11**	**C**
Q2	**B**	**Q7**	**B**	**Q12**	**B**
Q3	**C**	**Q8**	**B**	**Q13**	**B**
Q4	**B**	**Q9**	**B**	**Q14**	**B**
Q5	**B**	**Q10**	**A**	**Q15**	**B**

Answers: 1-B, 2-B, 3-C, 4-B, 5-B, 6-C, 7-B, 8-B, 9-B, 10-A, 11-C, 12-B, 13-B, 14-B, 15-B.