Materials Characterization

1. A solution containing 3.92 mg/100 mL of A (335g/mol) has a transmittance of 64.1% in a 1.5-cm cell at 425 nm. Calculate the molar absorptivity of A at this wavelength.

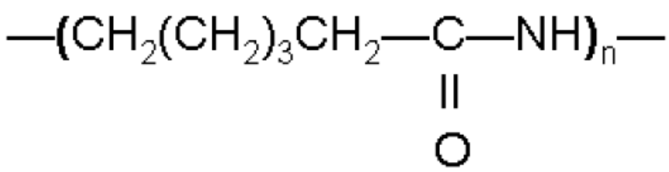
2. The following Raman data were obtained for $CHCl_3$ with the polarizer of the spectrometer set (1) parallel to the plane of polarization of the laser and (2) at 90 ° to the plane of the source.

	Relative Intensities		
	$\Delta\bar{\nu}$, cm^{-1}	(1) $I_{\parallel}$	(2) $I_{\perp}$
(a)	760	0.60	0.46
(b)	660	8.4	0.1
(c)	357	7.9	0.6
(d)	258	4.2	3.2

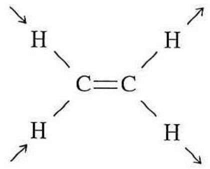
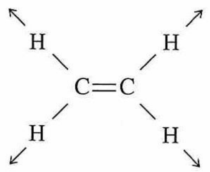
Calculate the depolarization ratio and indicate which Raman lines are polarized.

3. How many peaks are expected of C1s XPS spectra of Nylon 6?

Nylon 6



4. Indicate whether the following vibrations are active or inactive in the IR spectrum.

Molecule	Motion
(a) $CH_3—CH_3$	C—C stretching
(b) $CH_3—CCl_3$	C—C stretching
(c) SO_2	Symmetric stretching
(d) $CH_2=CH_2$	C—H stretching: 
(e) $CH_2=CH_2$	C—H stretching: 

5. (I) Express the following absorbances in terms of percent transmittance:
   (a)0.042 (b) 0.917 (c) 0.245
   (II) Convert the following transmittance data to absorbances:
   (d) 5.38% (e) 39.4%

6. Calculate the approximate wavenumber and wavelength of the fundamental absorption due to the stretching vibration of a carbonyl group C=O.

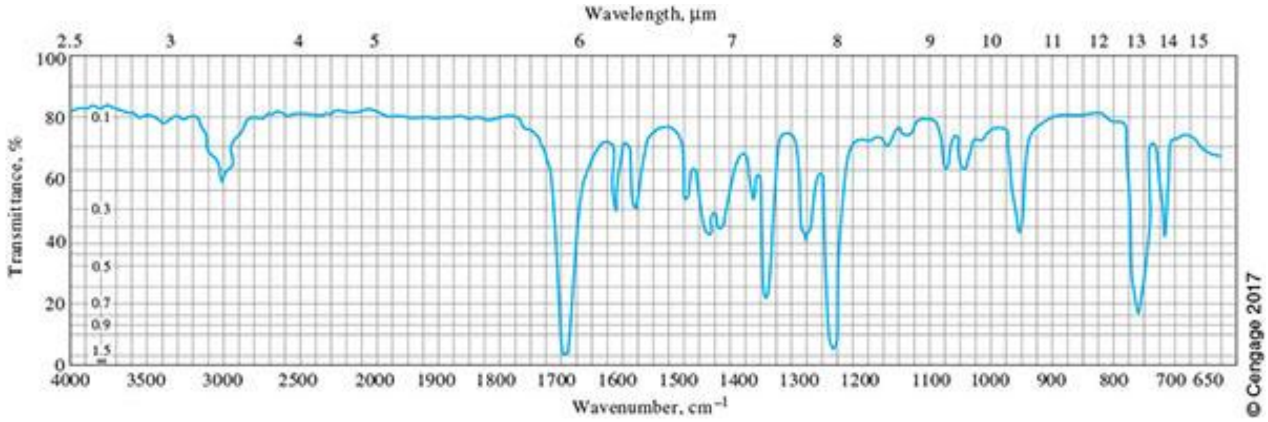
7. Calculate the absorption frequency corresponding to the –C-H stretching vibration treating the group as a simple diatomic C-H molecule with a force constant of $k=5.0x10^2 N/m$. Compare the calculated value with the range found in correlation charts.

8. The wavelength of the fundamental N-H stretching vibration is about 1.5 μm. What is the approximate wavenumber and wavelength of the first overtone peak for the N-H stretch?

9. Determine the index of hydrogen deficiency for each of the following compounds:

(a)C_8H_7NO (b) $C_3H_7NO_3$ (c) $C_4H_4BNO_2$ (d) $C_5H_3ClN_4$ (e) $C_{21}H_{22}N_2O_2$

10. The spectrum is that of a high boiling point liquid having the empirical formula $C_9H_{10}O$. Identify the compound as closely as possible.



11. Name the two most common types of scanning probe microscopes (a) How do they differ? (b) What are the advantages of each type? (c) What are the major limitations of each type?

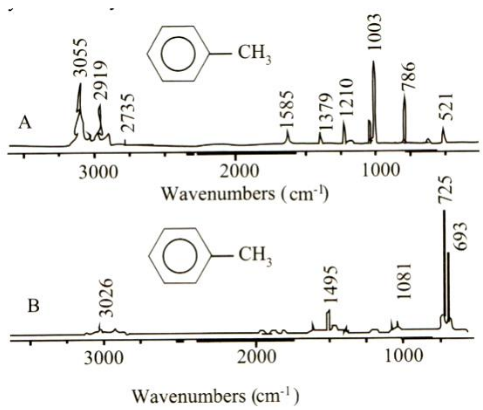
12. Describe the mechanism of the three modes in atomic force microscope (AFM)?

13. Describe the geometrical conditions for X-ray diffraction by a crystal in terms of vector of reciprocal lattices (d^*_{hkl}), Edward sphere and Debye-Scherrer rings?

14. Explain the broadening of the diffraction pattern in X-ray diffraction due to (1) cystallte size; (2) lattice distortion?

15. Please describe the mechanism difference of the following molecular spectroscopy. (a) FTIR; (b) Raman.

16. Following two spectra of toluene were acquired by Infrared and Raman spectrometry individually.



(1) Point out which one was obtained by Raman spectrometry. Explain

(2) What are the advantages of Raman spectroscopy compared to Infrared spectroscopy? State your reasons.

17. **(a)** Describe the mechanism of emitted (1s) electron in X-ray photoelectron spectroscopy (XPS) and how it is possible to distinguish between XPS and Auger electron peaks? **(b)** Describe the mechanism of the production of a KLM Auger electron and X-ray fluorescence (XRF) photon in Auger electron spectroscopy (AES)?

18. What is bright field (BF) and dark field (DF) in TEM?

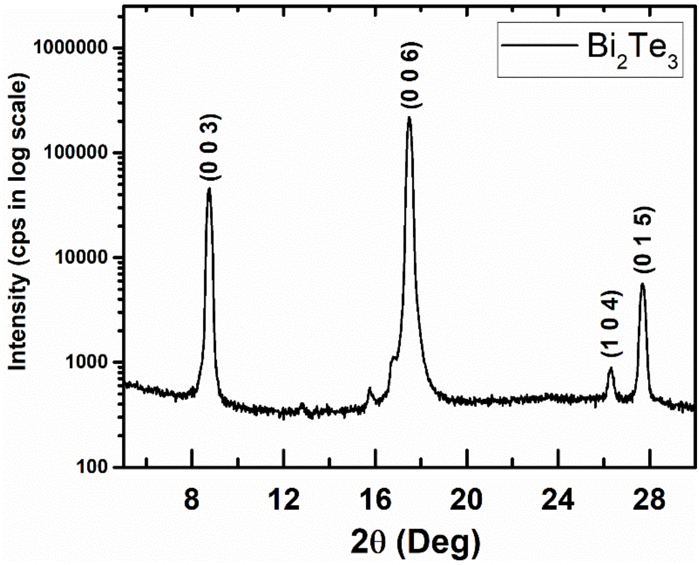
19. What is CuKα and Cu Lβ X-ray in EDS measurments?

20. The XRD pattern of a polycrystalline Bi_2Te_3 film is given in the Figure below. Known that Bi_2Te_3 has a hexagonal structure and the wavelength Cu K_α is 1.5406 Å.

(a) Fitting (0 0 6) peak with Psdvoigt1 function yielded x_c = 17.5 and w = 0.215. Calculate the grain size using the Scherrer equation.

(b) Calculate the d-spacing of (0 0 6) plane.

(c) Determine the c-axis lattice constant of Bi_2Te_3.



21.

(a) What is the basic working principle and the key components of a UV-Vis Spectroscopy?

(b) Present Tauc plot for determining the optical band gap for direct and indirect band gap materials.

(c) What is the basic working principle and the key components of Fourier Transform Infrared (FTIR) Spectroscopy?

(d) Explain both positive and negative aspects of (a) Raman Spectroscopy, and (b) X-Ray techniques.

22. For electrical properties measured by the Hall effect method, the sheet resistance of a film is 290.2 Ω/sq, the sheet carrier concentration is 9.992×10^{14} cm^{-2}, and the film thickness is 140nm, carrier mobility is 21.5 cm^2/Vs. Calculate the resistivity, carrier concentration, and conductivity of the film.

23. For the nanoindentation technique, present the following things:

(a) Draw a typical load vs. displacement curve.

(b) Write the formula for calculating the hardness, reduced modulus, and young modulus using the Oliver and Pharr method.

(c) Given a nanoindentation result for a SnO_2 film using an ideal Berkovich indenter that maximum force is 473.7 μN, maximum depth is 80.4 nm, and contact stiffness is 21.7 μN/nm. Calculate the hardness and reduced modulus of the film.

24. SEM and XPS methods

(a) Present briefly the structural and working principles of SEM

(b) Present the Spin-Orbital angular momentum, and write the area relationships for:

(i) $p_{1/2} : p_{3/2} = ?$ (ii) $d_{3/2} : d_{5/2} = ?$ (iii) $f_{5/2} : f_{7/2} = ?$

(c) In an XPS experiment, the integrated peak area of the C 1s signal at 285 eV is $I_C =$ 5000 counts, and the corresponding sensitivity factor $S_C = 1.0$. The O 1s peak at 531 eV has an integrated area of I_O =3000 counts I_O = 3000 counts, with a sensitivity factor S_O =2.93. Calculate the atomic concentration of carbon and oxygen in the sample.

25.**TEM method**

(a) What is the basic working principle of Transmission Electron Microscopy (TEM)?

(b) What are the main components of a Transmission Electron Microscope (TEM)?

(c) What factors affect the resolution in a TEM?

(d) How is contrast generated in a TEM image?

(e) What are the limitations of TEM?

26. Photoluminescence (PL) method

(a) What is the basic working principle of Photoluminescence (PL) spectroscopy?

(b) What are the main components of a Photoluminescence (PL) spectroscopy setup?

(c) How is Photoluminescence (PL) spectroscopy used to determine the bandgap of a material?

(d) What factors influence the intensity and spectral shape of the Photoluminescence (PL) signal?

(e) What are the limitations of Photoluminescence (PL) spectroscopy in material analysis?

27. Corrosion basics

(a) What is the fundamental principle behind corrosion in electrochemical terms?

(b) What is the role of the electrochemical cell in studying corrosion?

(c) How does Tafel analysis help in understanding the corrosion rate?

(d) What is the significance of Electrochemical Impedance Spectroscopy (EIS) in corrosion studies?

28. Thermal analysis

(a) What is the basic working principle of Thermal Analysis methods of Differential Scanning Calorimetry (DSC) and Thermogravimetric Analysis (TGA)?

(b) What are the key components of Differential Scanning Calorimetry (DSC) instrumentation?

(c) How is data from Thermogravimetric Analysis (TGA) interpreted?

29. Solve the following quantitative problems

(a) A cubic crystal has a prominent XRD peak at a diffraction angle (2θ) of 44.5° when using Cu Kα radiation (λ = 1.5406 Å). Calculate the lattice parameter a of the crystal. Assume the peak corresponds to the (110) plane.

(b) A material exhibits an XRD peak at 2θ = 30° with a full width at half maximum (FWHM) of 0.2° using Cu Kα (λ = 1.5406 Å). Calculate the crystallite size D using the Scherrer equation.

(c) A molecule exhibits a Raman shift at 1580 cm^{-1}. Calculate the energy of this vibrational mode in electron volts (eV).