

IMPERIAL COLLEGE LONDON

M.Eng EXAMINATION IN CHEMICAL ENGINEERING 2020

PART III and IV

and

M.Sc. in ADVANCED CHEMICAL ENGINEERING

For Internal Students of Imperial College London

This paper is also taken for the relevant examination  
for the Associateship

**PRODUCT CHARACTERISATION**

**Wednesday 29<sup>th</sup> April 2020: 10:00 - 11:30**

Answer all three questions

**THIS EXAMINATION PAPER HAS SIX PAGES IN TOTAL  
WHICH INCLUDES THIS COVER SHEET**

Question 1 carries 25 marks

Question 2 carries 35 marks

Question 3 carries 40 marks

TURN OVER FOR QUESTION

### Question 3

[40 marks]

- (a) **Sketch** the Infrared and Raman spectra of liquid CO<sub>2</sub>. **Provide** notations for the axes; **indicate** the approximate positions of the spectral bands and briefly **explain** the origin of these spectral bands.

[10 marks]

- (b) The <sup>56</sup>FeH diatomic molecule absorbs infrared light having a wavenumber of 1661.0 cm<sup>-1</sup>. **Calculate** the wavenumber and frequency of light that <sup>54</sup>FeH would absorb. You may assume that mass of hydrogen atom is one atomic mass unit; velocity of light (*c*) = 2.998 × 10<sup>8</sup> m s<sup>-1</sup>.

[5 marks]

- (c) **Write** the expression for the Beer-Lambert Law in infrared absorption spectroscopy and **define** every term. The molar absorption coefficient (molar absorptivity) for an infrared band of a dye dissolved in 200 micrometres thick polymer film is 0.5 × 10<sup>6</sup> cm<sup>2</sup> mol<sup>-1</sup>. The measured absorbance of this band is 0.1. **Calculate** the concentration of the dye in the polymer film.

[5 marks]

- (d) How would you measure the distribution of substances during tablet dissolution using FTIR spectroscopic imaging? **Describe** the approach and relevant phenomena that can be studied using this approach. **Provide** approximate values for measured areas that can be analysed by this approach. **Support** your explanation with corresponding schematics and equations as appropriate.

[10 marks]

- (e) Which spectroscopic technique would you use to differentiate single-walled carbon nanotubes of different diameters? **Explain** why.

[10 marks]

END OF QUESTION 3

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**PRODUCT CHARACTERISATION**

**Thursday 6<sup>th</sup> May 2021: 10:00 - 11:30**

Answer all three questions

**THIS EXAMINATION PAPER HAS FIVE PAGES IN TOTAL  
WHICH INCLUDES THIS COVER SHEET**

Question 1 carries 30 marks

Question 2 carries 30 marks

Question 3 carries 40 marks

TURN OVER FOR QUESTION

### Question 3

[40 marks]

Vibrational spectroscopy is a major tool for characterising materials and products:

- (a) Providing brief explanations for your selections, **indicate** which of the following 4 molecules,  $^{37}\text{Cl}^{35}\text{Cl}$ ,  $\text{H}-\text{C}\equiv\text{N}$  (hydrogen cyanide),  $\text{C}_{60}$  fullerene and  $\text{H}_2\text{O}$  may show:
- Infrared absorption spectra?
  - Raman spectra?
  - Calculate the number of normal vibrations for each molecule.

[12 marks]

- (b) Diffraction of visible or infrared light is the reason for a limited spatial resolution in the studies materials or products by Raman or Infrared spectroscopy combined with corresponding microscopes. **Describe** two approaches of overcoming diffraction limit to achieve high spatial resolution in Raman and Infrared spectroscopic imaging. **Provide** corresponding equations/schematics and examples of samples where such high spatial resolution was useful.

[13 marks]

- (c) **Explain** the differences between Attenuated Total Reflection (ATR)–FTIR spectroscopy and confocal Raman microscopy when using these techniques to probe depths into polymeric samples. **Explain** how the range of the probing depth can be changed when using each of these approaches. **Support** your answers with corresponding equations or/and schematics as appropriate.

[15 marks]

END OF PAPER

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**PRODUCT CHARACTERISATION**

**Monday 9<sup>th</sup> May 2022: 10:00 – 11:30**

Answer all three questions

**THIS EXAMINATION PAPER HAS SIX PAGES IN TOTAL  
WHICH INCLUDES THIS COVER SHEET**

Question 1 carries 20 marks

Question 2 carries 40 marks

Question 3 carries 40 marks

TURN OVER FOR QUESTION

### Question 3

[40 marks]

Vibrational spectroscopy is a major tool for characterising materials and products:

- (a) Based on the understanding of Infrared and Raman spectroscopy, and Hooke's law **arrange** the following stretching vibrations of functional groups in increasing order for their wavenumber, so lowest wavenumber ranks first. **Explain** your answers briefly:

(i) C-H                      (ii) C-F                      (iii) N-H                      (iv) O-H

[8 marks]

- (b) For the polymeric sample analysed by Attenuated Total Reflection (ATR-FTIR) spectroscopy, (C=O) band has a depth of penetration equal to 3  $\mu\text{m}$ . **Calculate** the depth of penetration for the C-O bond.

[5 marks]

- (c) Carbon tetrachloride ( $\text{CCl}_4$ ) has 3 Raman-active vibrations that occur at 218, 314 and 459  $\text{cm}^{-1}$  away from the laser line. Draw a demonstration of the Raman spectrum of  $\text{CCl}_4$  that includes both the Stokes and anti-Stokes lines with a **brief explanation**. **Explain** why the anti-Stokes bands of  $\text{CCl}_4$  have the following order of intensity:  $218 > 314 > 459 \text{ cm}^{-1}$ .

[13 marks]

- (d) **Explain** how the high spatial resolution achieved with micro ATR-FTIR spectroscopic imaging. **Compare** this spatial resolution with the spatial resolution achieved in FTIR spectroscopic imaging in transmission and **explain** the difference. **Explain** how the spatial resolution in transmission may be increased. **Support** your answers with corresponding equations or/and schematics as appropriate.

[14 marks]

END OF QUESTION 3

END OF PAPER