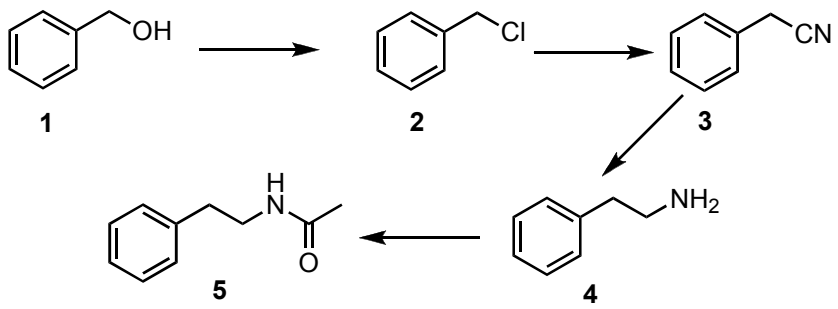
Chemistry 30B Discussion - Week 2: IR Spectroscopy - DCF

1: Matching compounds to spectra

a) Research assistant Bill Jones has carried out the following synthetic sequence, but he stored the compounds in unlabelled bottles.



When his research advisor finds out what he has done, he tells him to take IR spectra of the five compounds. Help Billy identify which bottles contain which compounds using *Spectra set I*. Label the important peaks with their corresponding functional groups as justification of your assignments.

Spectrum **A** is of compound _____

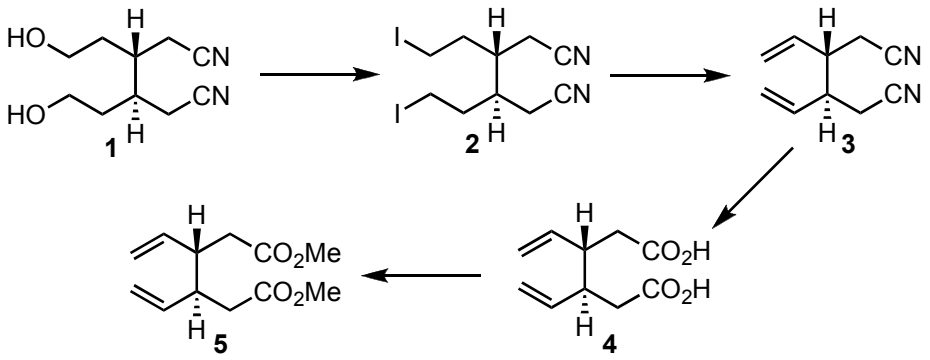
Spectrum **B** is of compound _____

Spectrum **C** is of compound _____

Spectrum **D** is of compound _____

Spectrum **E** is of compound _____

b) As in **a**, use the IR spectra provided in *Set II* and match them with each of the numbered intermediates in the reaction scheme below. Don't forget to label the spectra with the relevant functional groups.



Spectrum **A** is of compound _____

Spectrum **B** is of compound _____

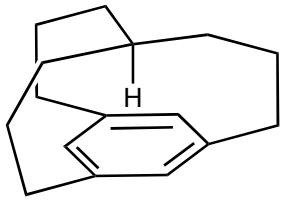
Spectrum **C** is of compound _____

Spectrum **D** is of compound _____

Spectrum **E** is of compound _____

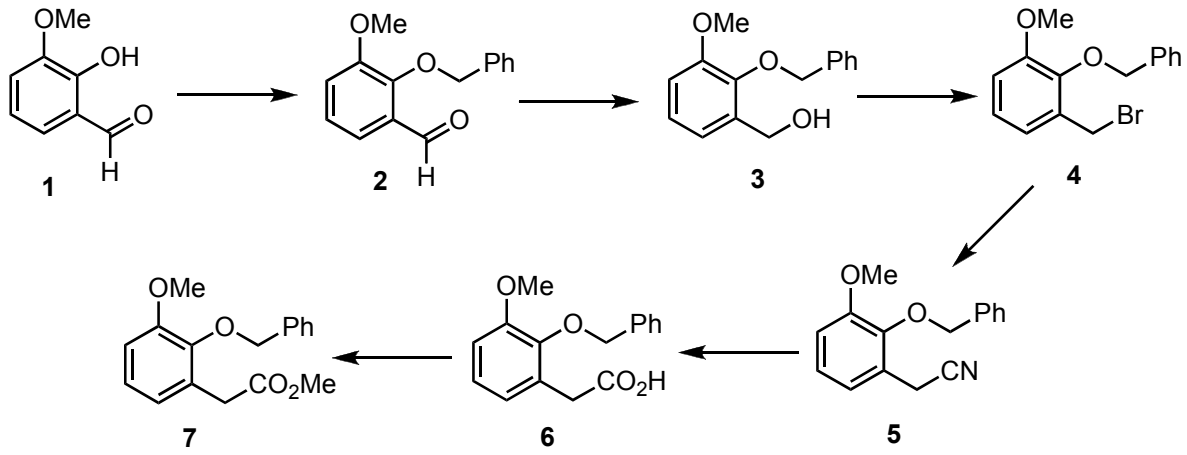
2: Explain the following observation (Challenging question)

The cyclophane below, in addition to the usual C-H stretches at 2900-3100 cm-1, it also shows a very unusual C-H stretch at 3325 cm-1. Explain this observation.



3: Predicting unique features in IR

You are given the following synthetic intermediates from a lab mate, but the labels are totally illegible.



To help identify which bottles contain which compounds you will use IR spectroscopy. Before you take the spectra, your research adviser wants to know what features of the IR spectrum of each compound would uniquely distinguish it from the others. Compile the list below.

Unique features of **1**: _____

Unique features of **2**: _____

Unique features of **3**: _____

Unique features of **4**: _____

Unique features of **5**: _____

Unique features of **6**: _____

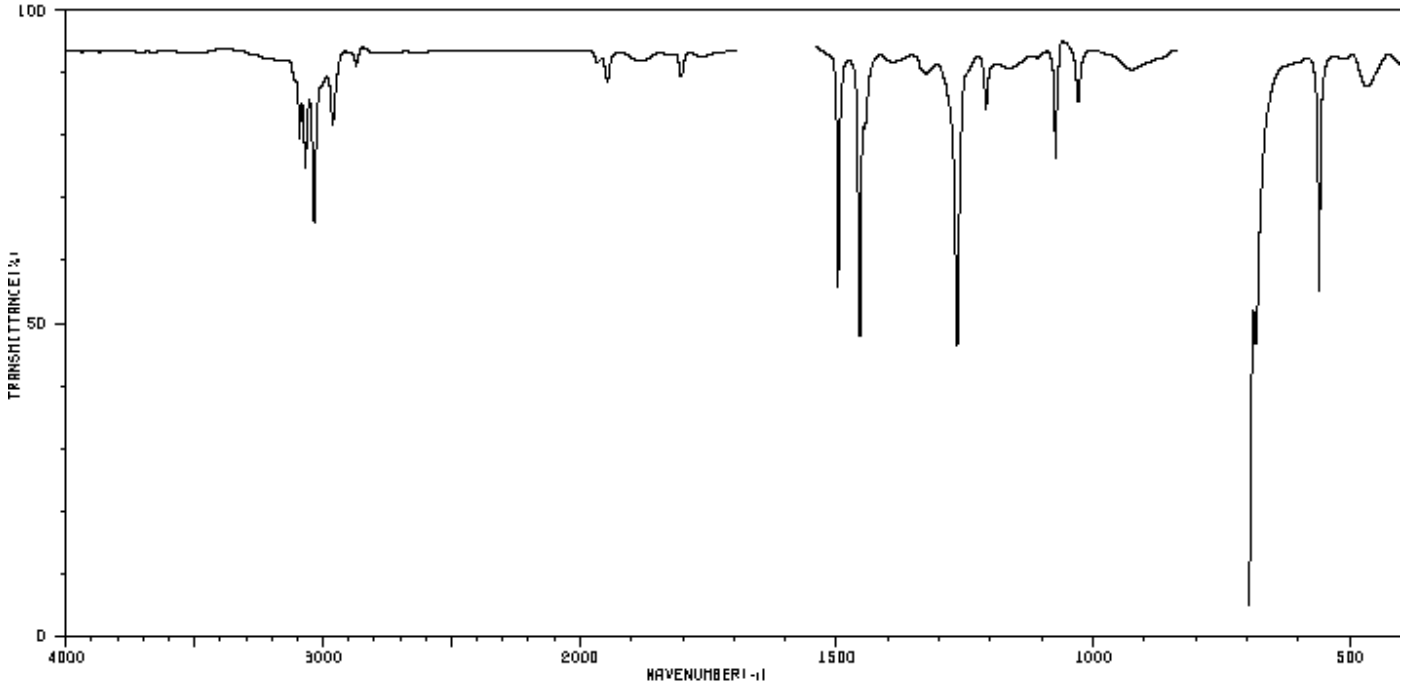
Unique features of **7**: _____

Book Problems:

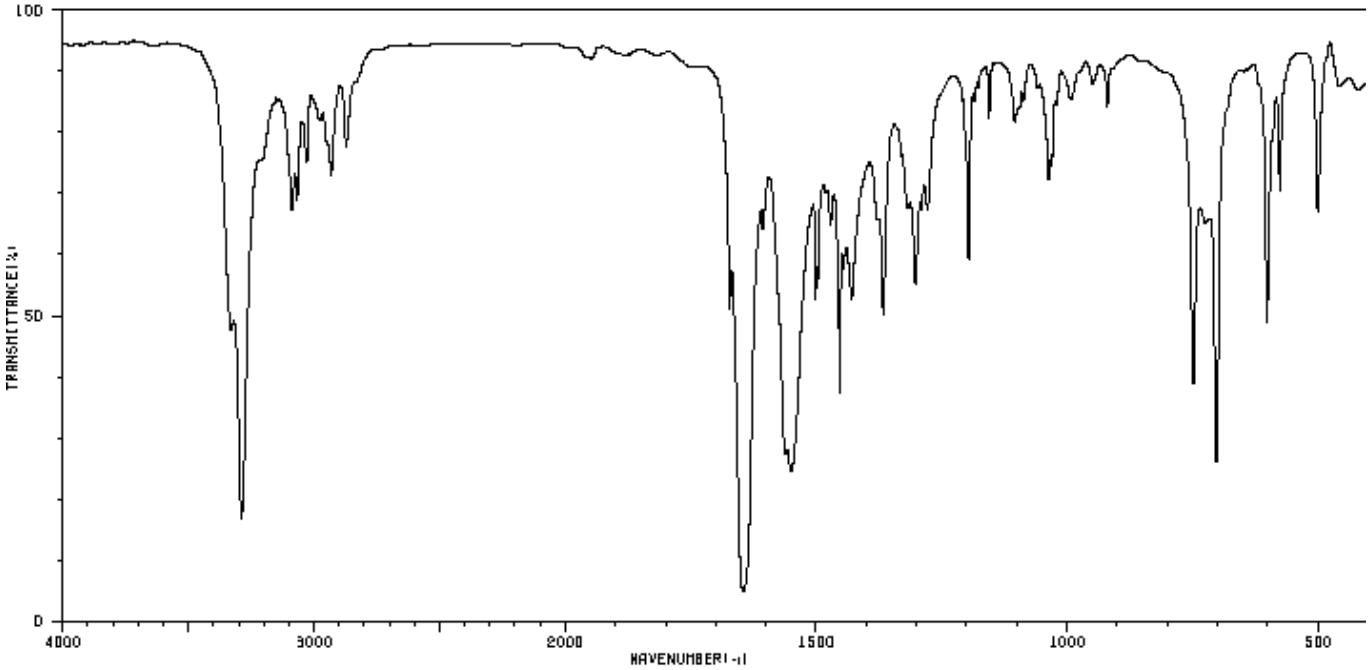
Chapter 12: Problems 4, 8, & 11(h)

Spectra Set I:

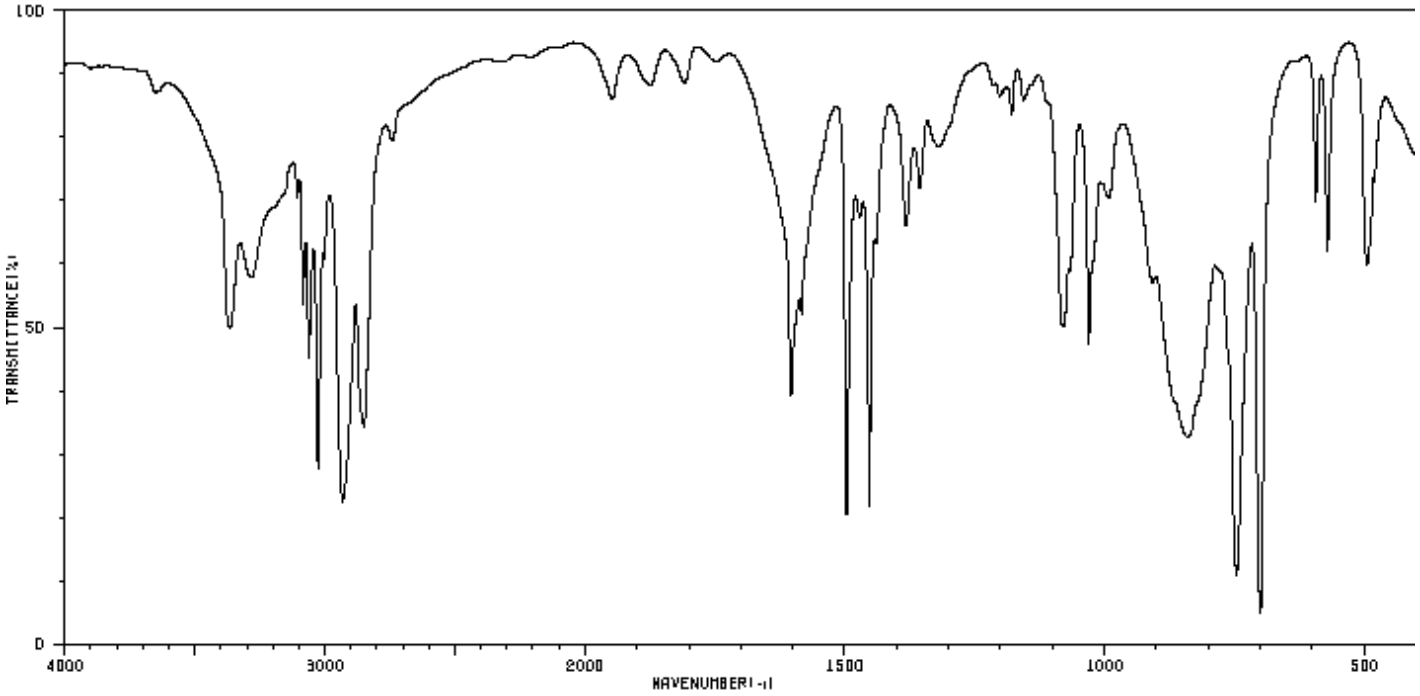
I-A



I-B



I-C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50
0
TRANSMITTANCE[%]
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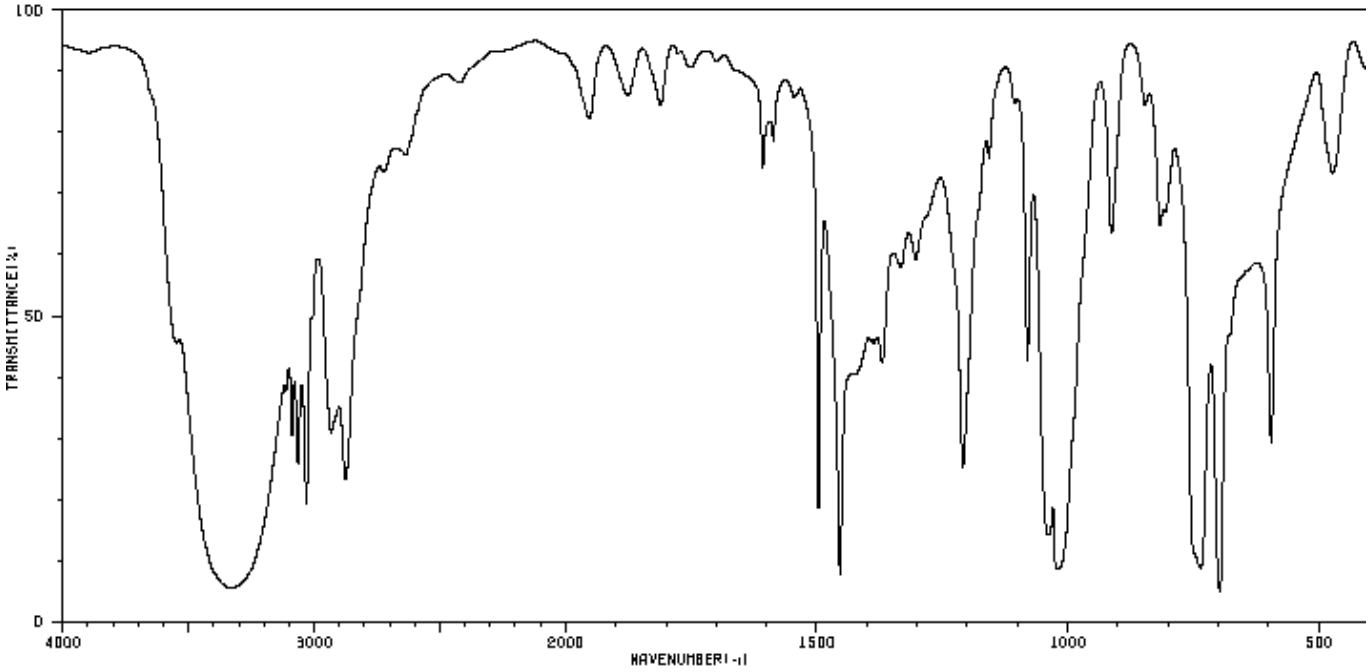
3000
2000
1500
1000
500
WAVENUMBER[-1]

I-D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TRANSMITTANCE[%]
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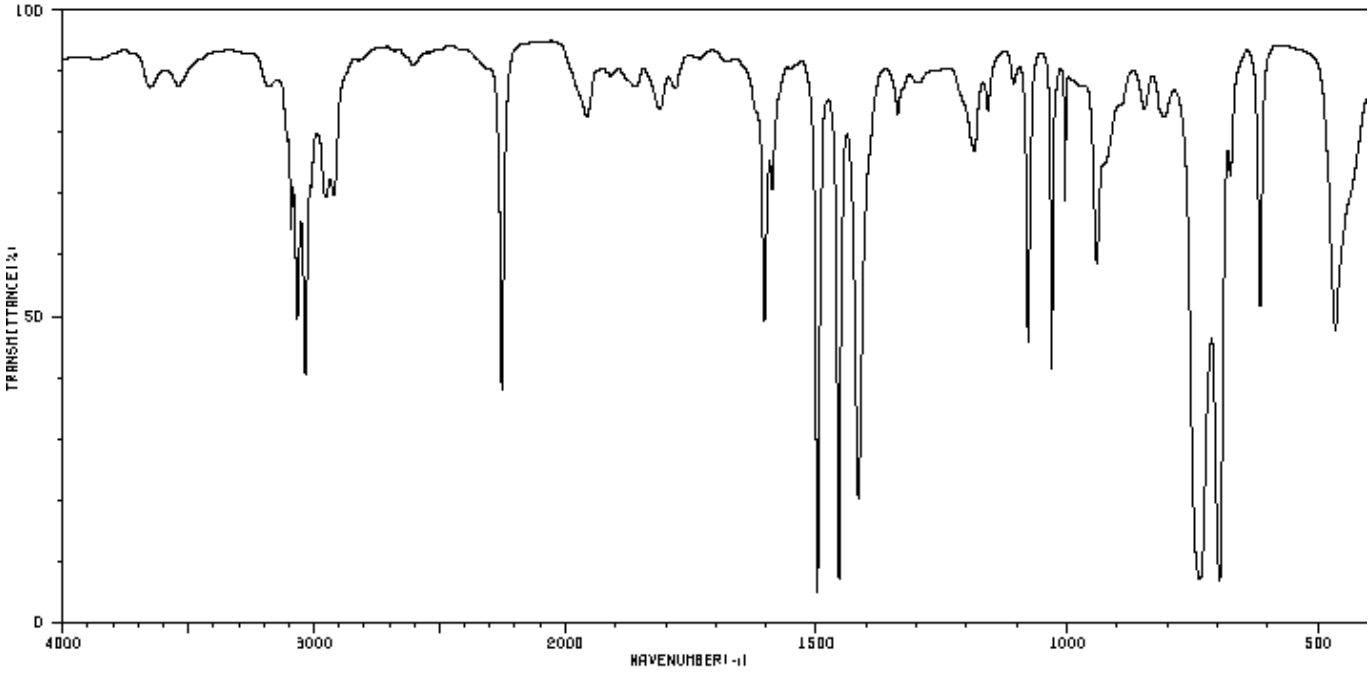
WAVENUMBER[-1]

I-E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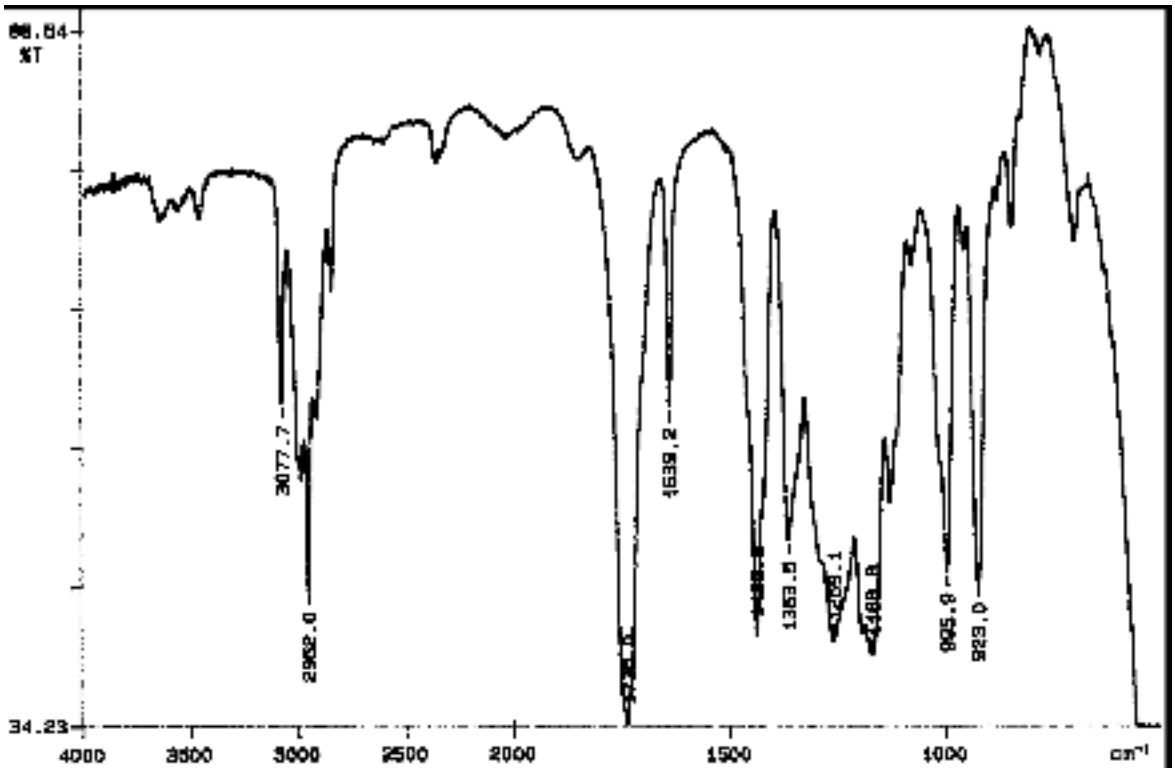
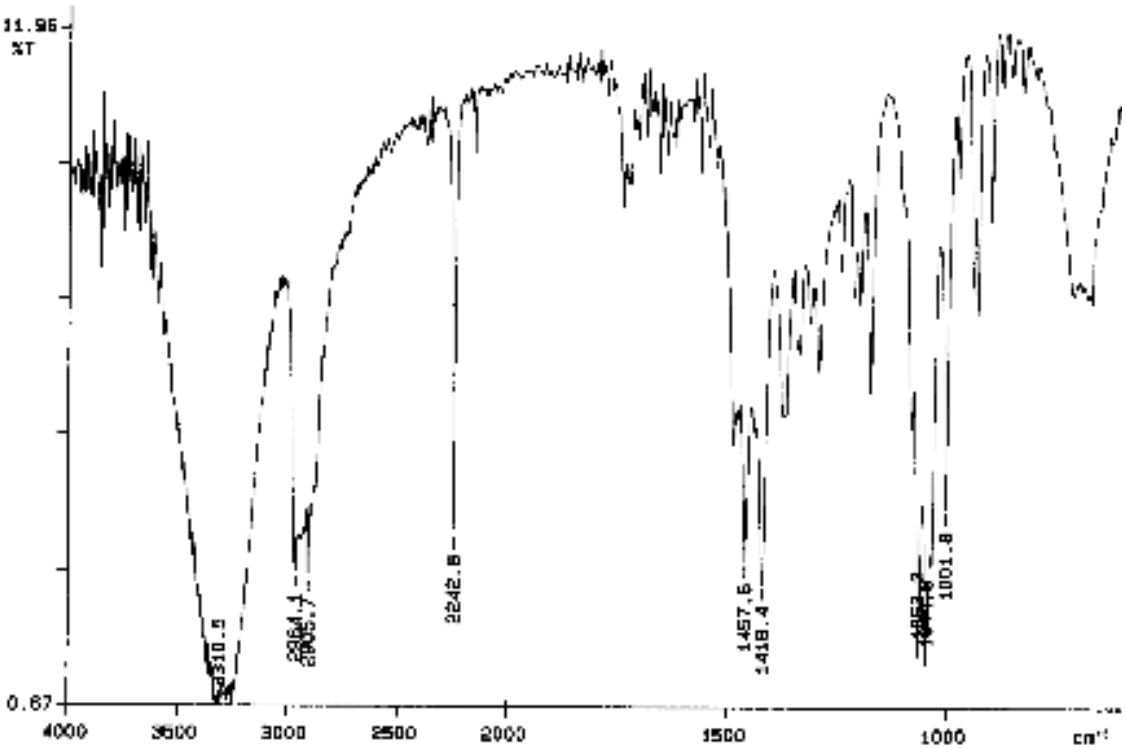
WAVENUMBER[-1]

Spectra Set II:

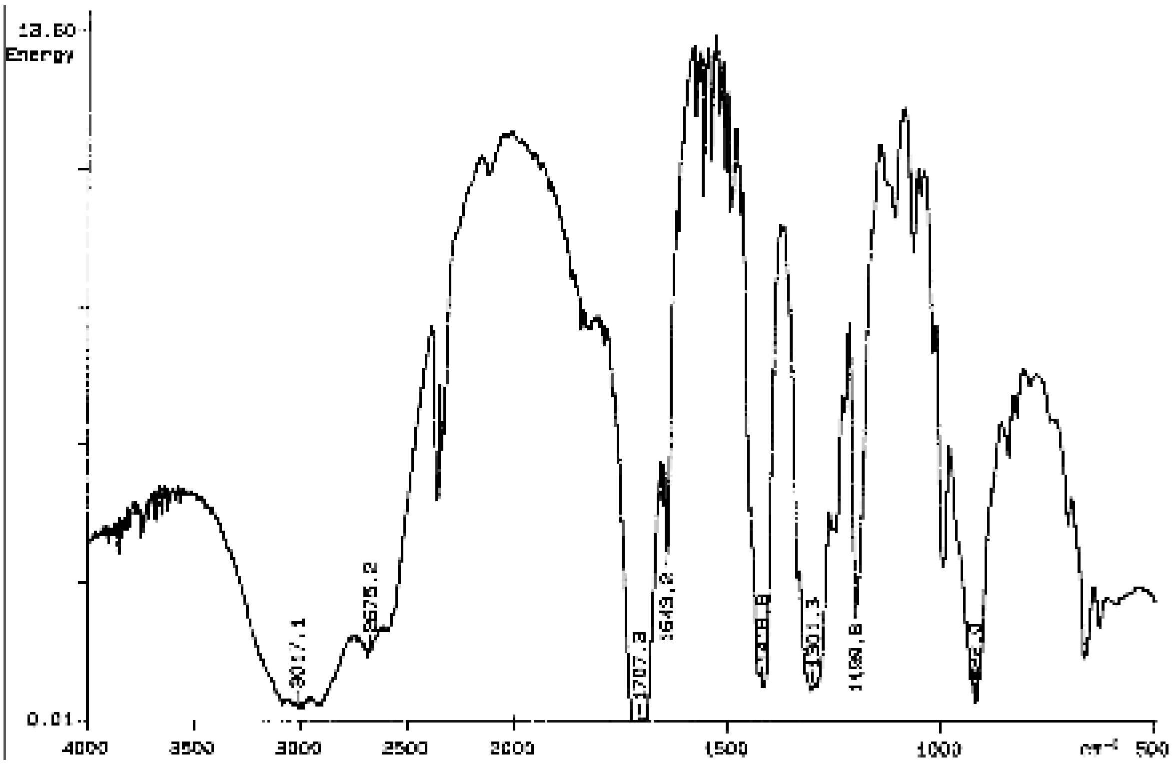
II-A



II-B



II-C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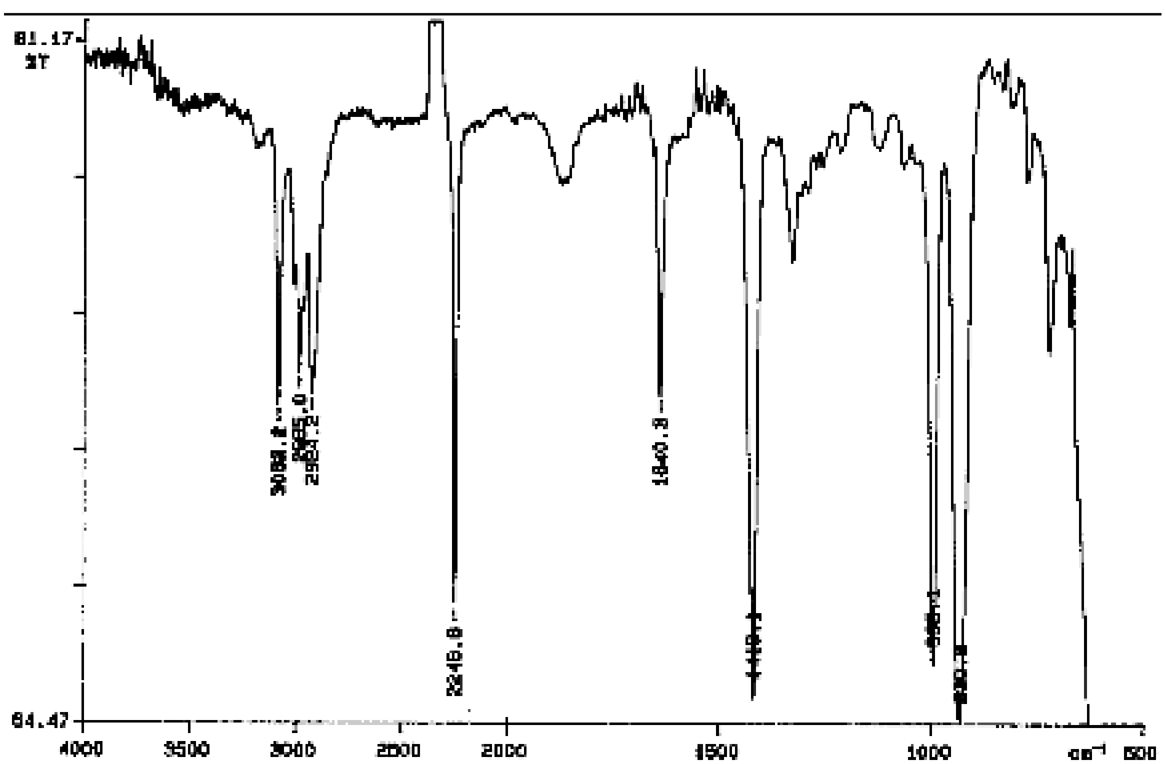
1649.2
1301.3

II-D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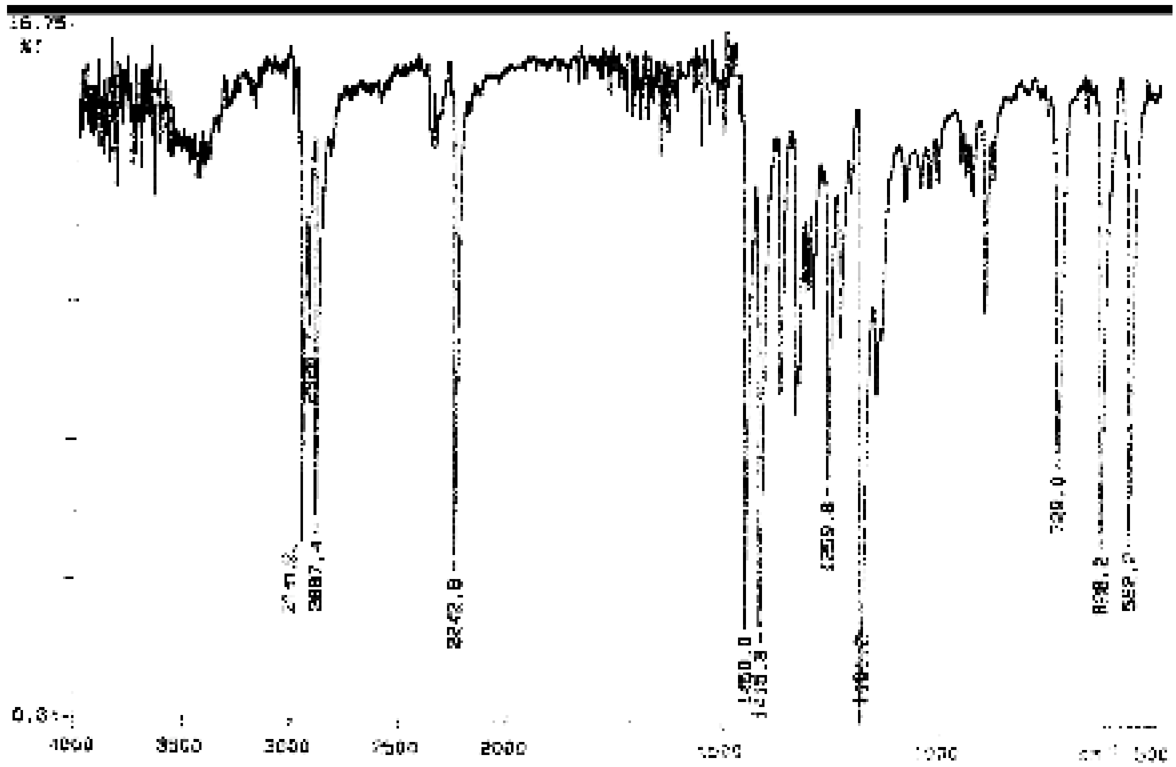
II-E



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%T
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1000
500
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2242.8
1259.8