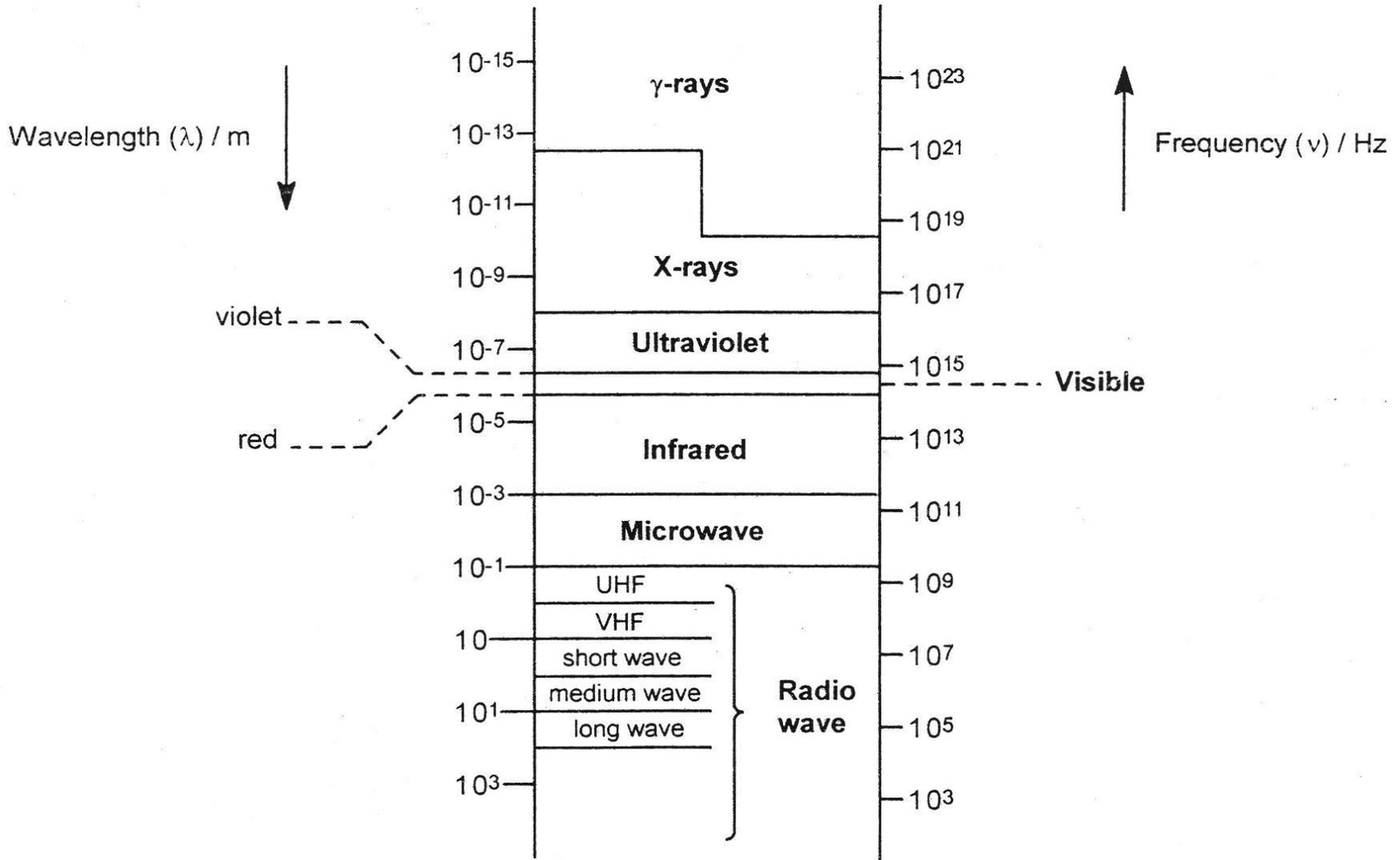




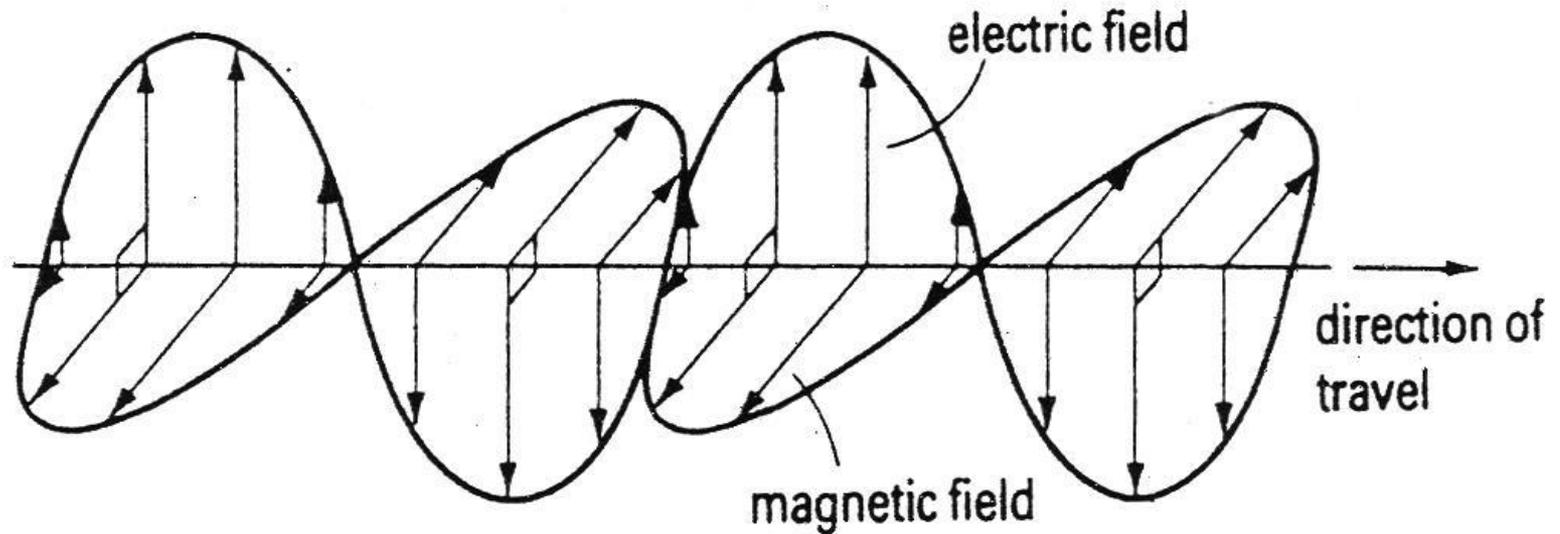
[WWW.CHEMSHEETS.CO.UK](http://www.chemsheets.co.uk)

IR SPECTROSCOPY

Electromagnetic spectrum



- Light is one form of electromagnetic radiation.
- Light is only a very small part of the electromagnetic spectrum.
- Electromagnetic waves consist of electric and magnetic fields which are perpendicular to each other and to the direction of travel of the wave.
- The electric and magnetic fields vibrate at the same frequency as each other.

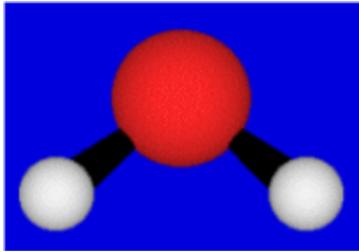


- Atoms, molecules and ions can absorb (or emit) electromagnetic radiation of specific frequencies, and this can be used to identify them.

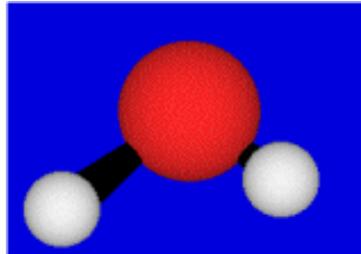
| Electromagnetic radiation absorbed | What the energy is used for | Spectroscopy technique |
|---|---|-------------------------------------|
| Ultra-violet / visible | Movement of electrons to higher energy levels | Ultra-violet / visible spectroscopy |
| Infra-red | To vibrate bonds | Infra-red spectroscopy |
| Microwaves | To rotate molecules | Microwave spectroscopy |
| Radio waves | To change nuclear spin | NMR spectroscopy |

Bond vibrations

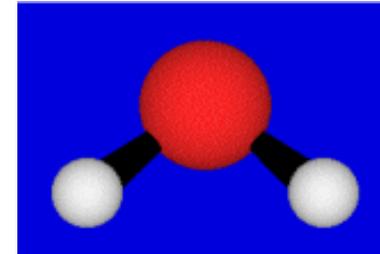
- All bonds vibrate at a characteristic frequency.
- There are different types of vibration.



Symmetric stretch



Assymmetric stretch



Bending

- The frequency depends on the mass of the atoms in the bond, the bond strength, and the type of vibration.
- The frequencies at which they vibrate are in the infra-red region of the electromagnetic spectrum.

IR Spectra

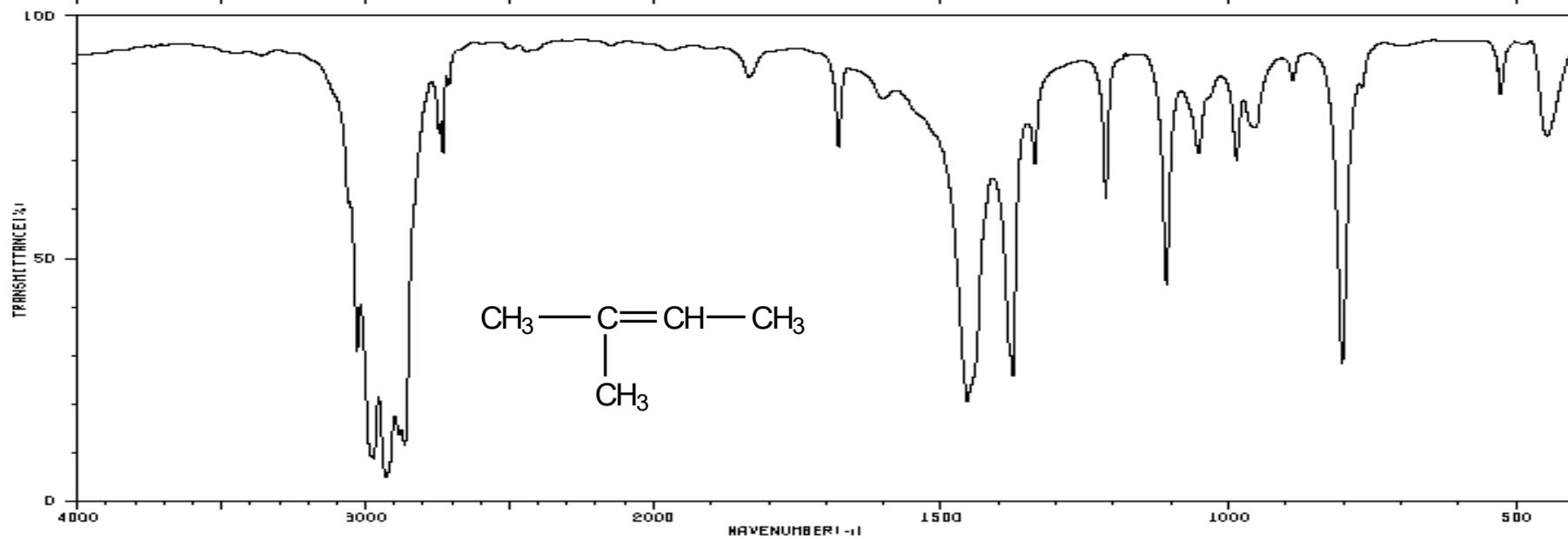
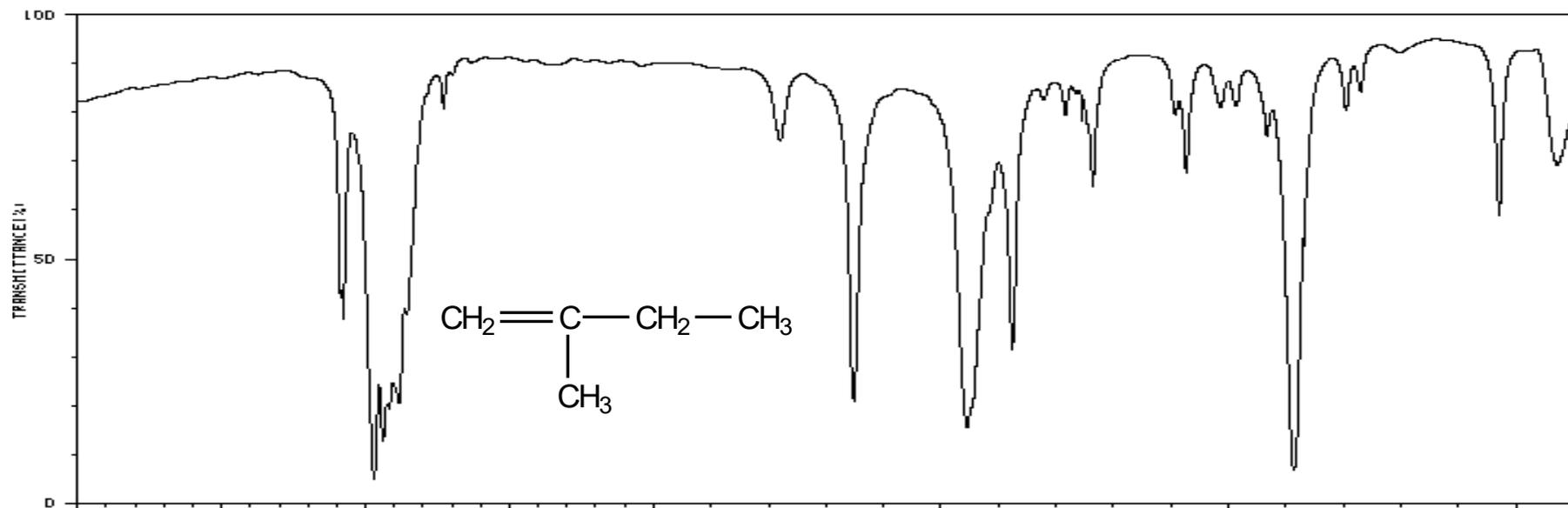
- If IR light is passed through the compound, it will absorb some or all of the light at the frequencies at which its bonds vibrate.
- Wavenumbers (cm^{-1}) are used as a measure of the wavelength or frequency of the absorption.

$$\text{Wavenumber} = \frac{1}{\text{wavelength (cm)}}$$

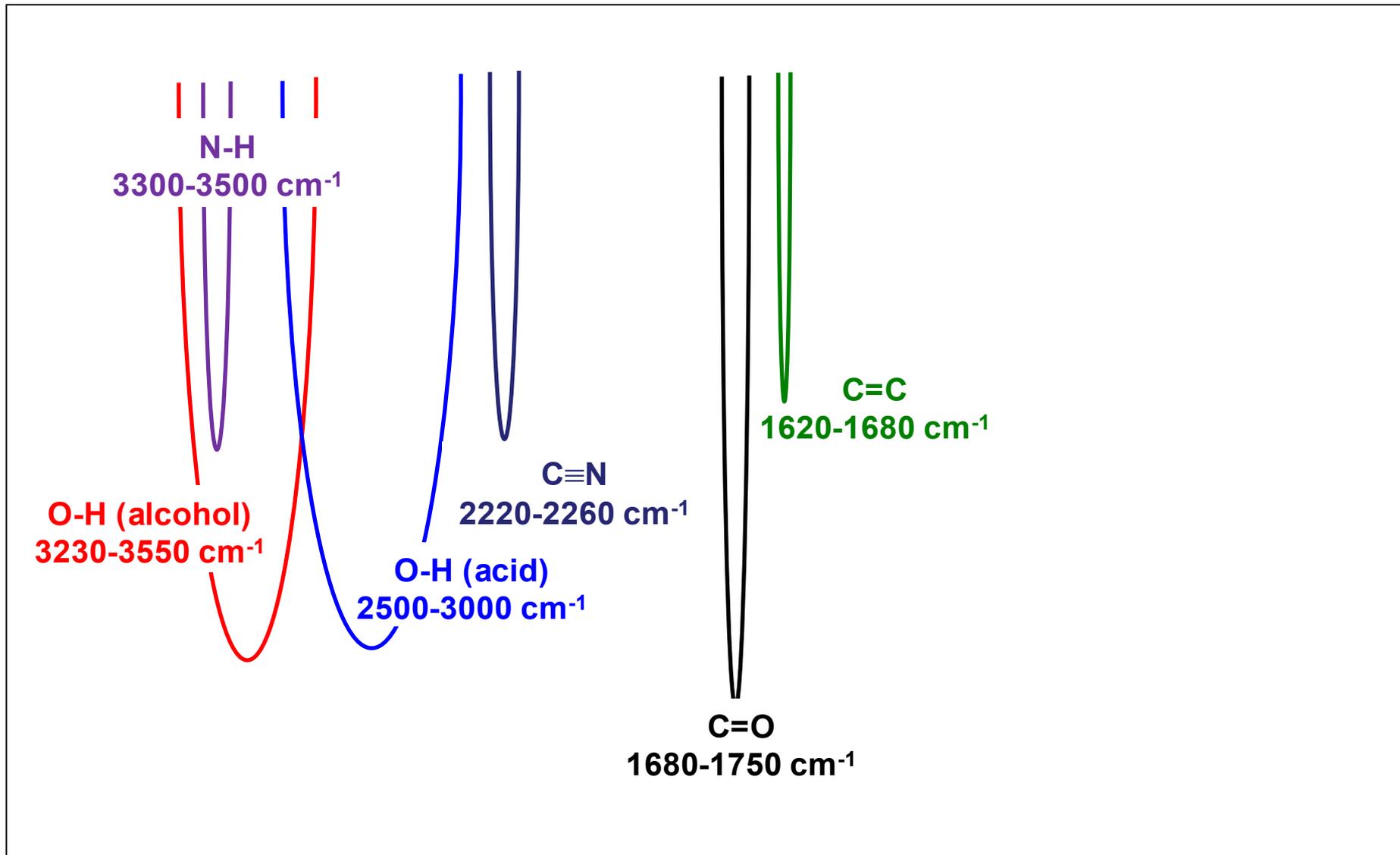
- IR light absorbed is in the range $4000 - 400 \text{ cm}^{-1}$.
- Above 1500 cm^{-1} is used to identify functional groups.
- Below 1500 cm^{-1} is used for fingerprinting.

Fingerprinting (below 1500 cm^{-1})

- Complicated and contains many signals – picking out functional group signals difficult.
- This part of the spectrum is unique for every compound, and so can be used as a "fingerprint".
- This region can also be used to check if a compound is pure.



Functional Groups (above 1500 cm^{-1})



4000

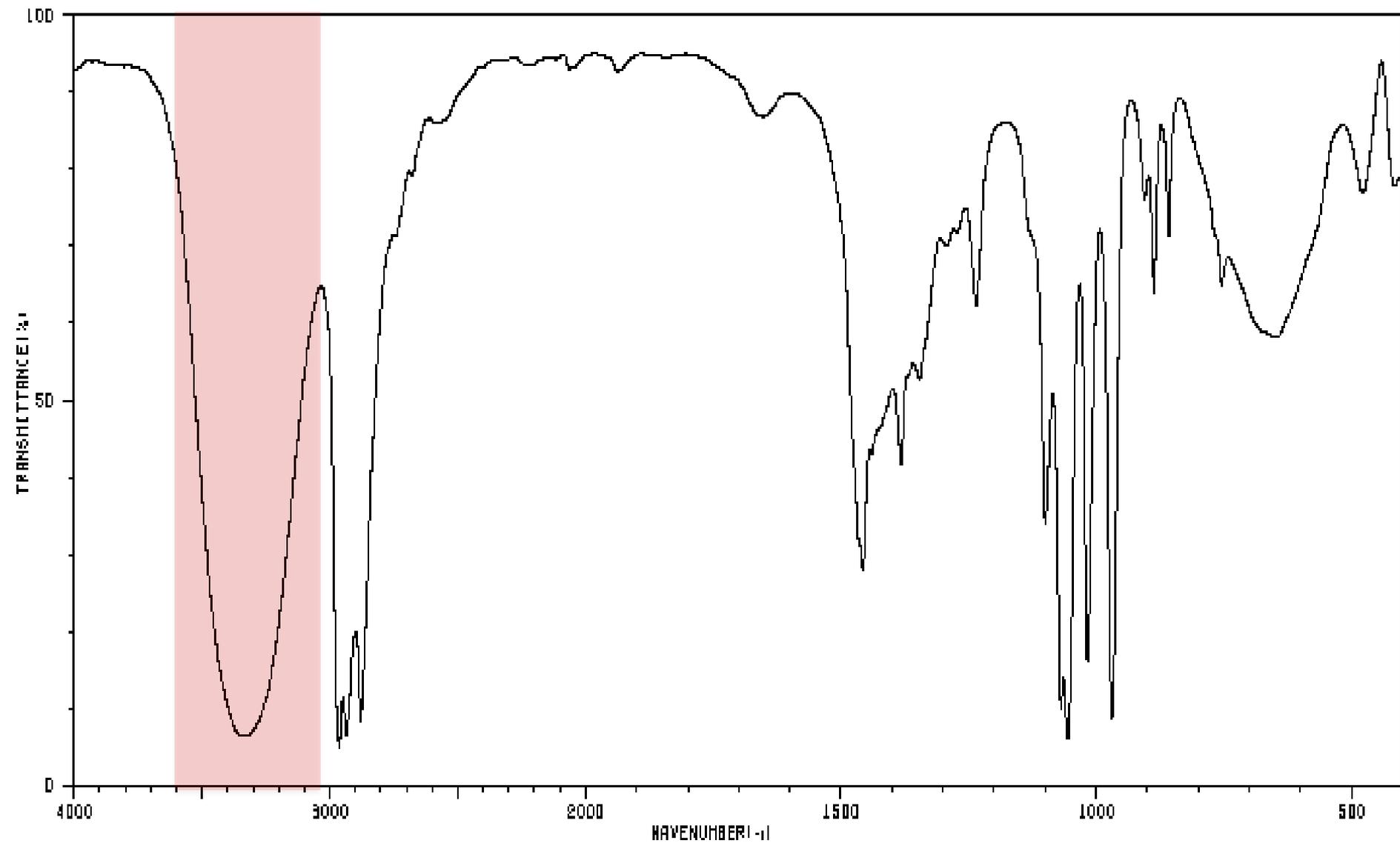
3000

2000

1500

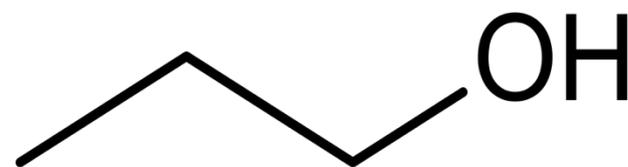
1000

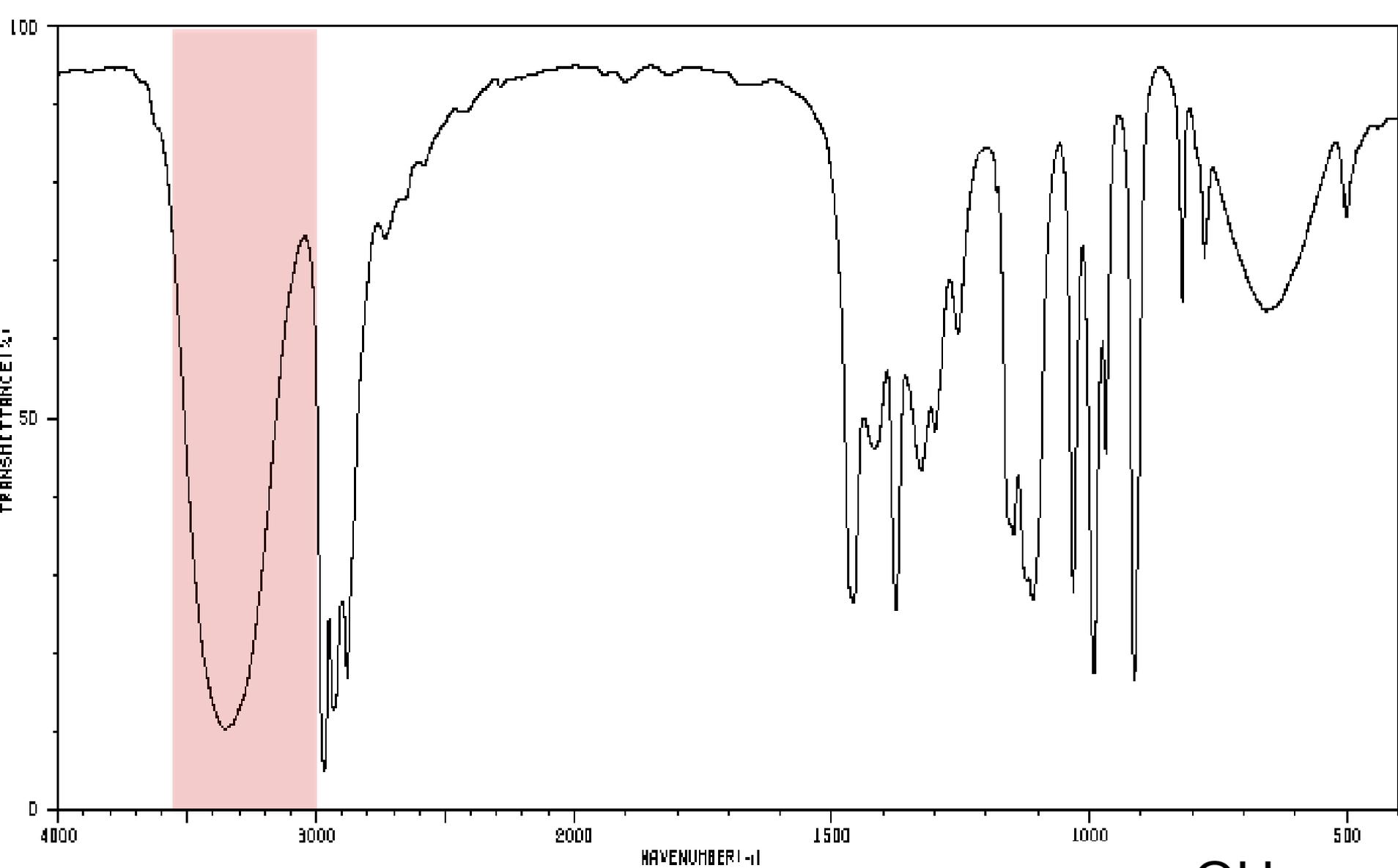
500



Alcohol O-H

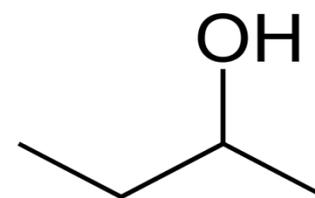
propan-1-ol

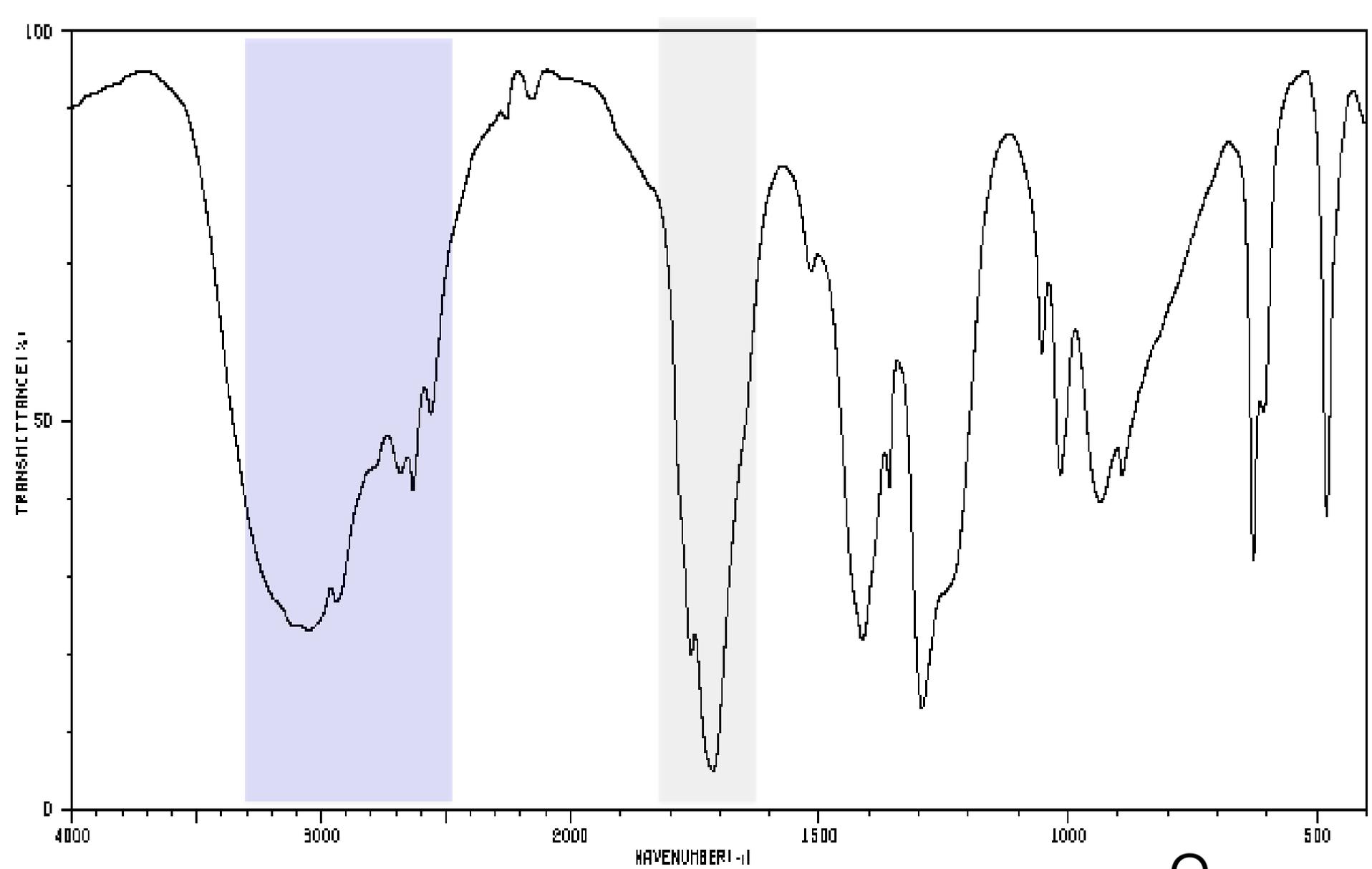




Alcohol O-H

butan-2-ol

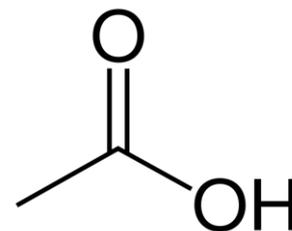


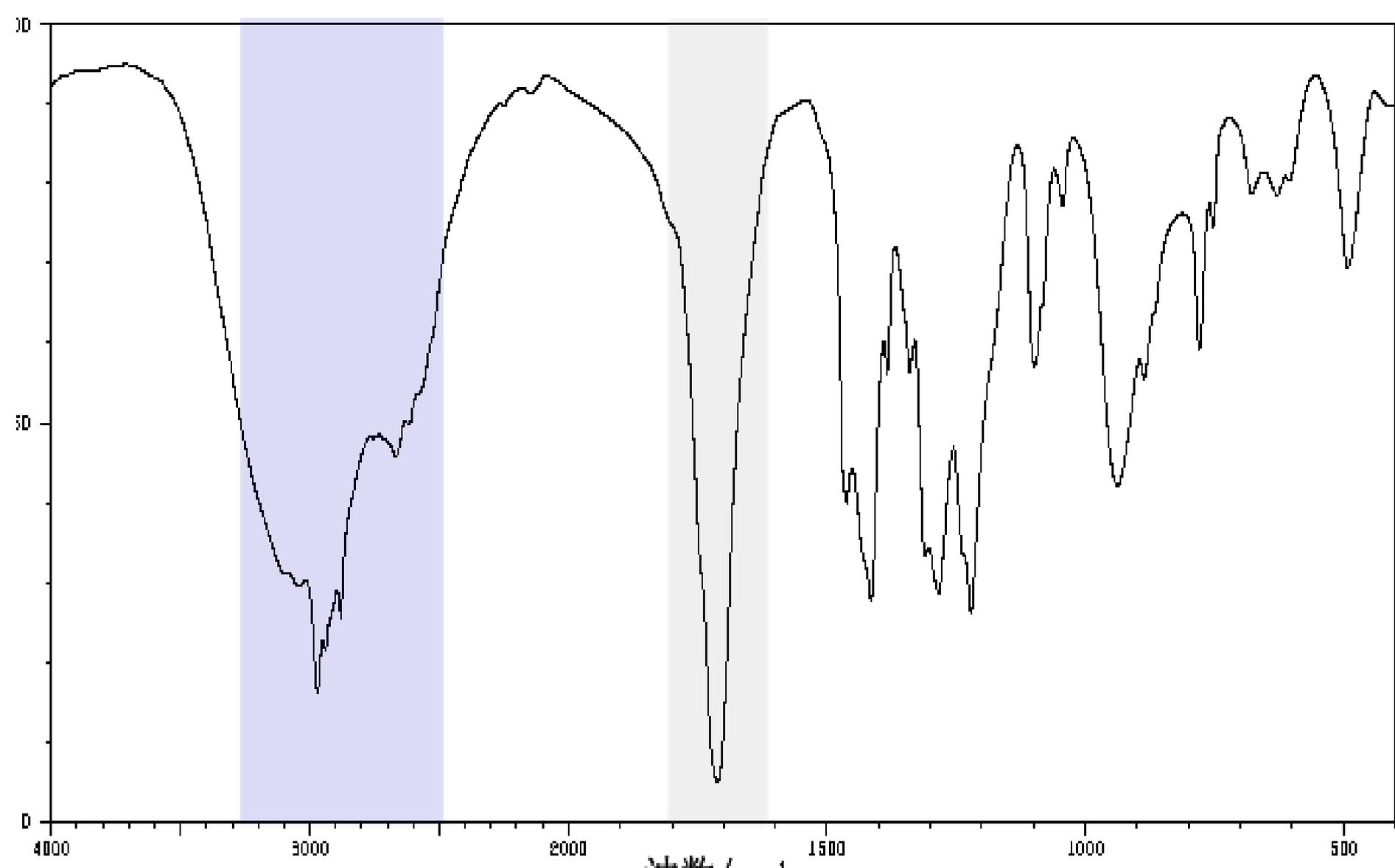


Acid O-H

C=O

ethanoic acid

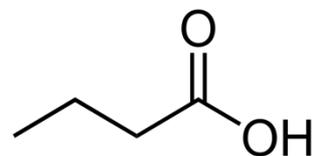


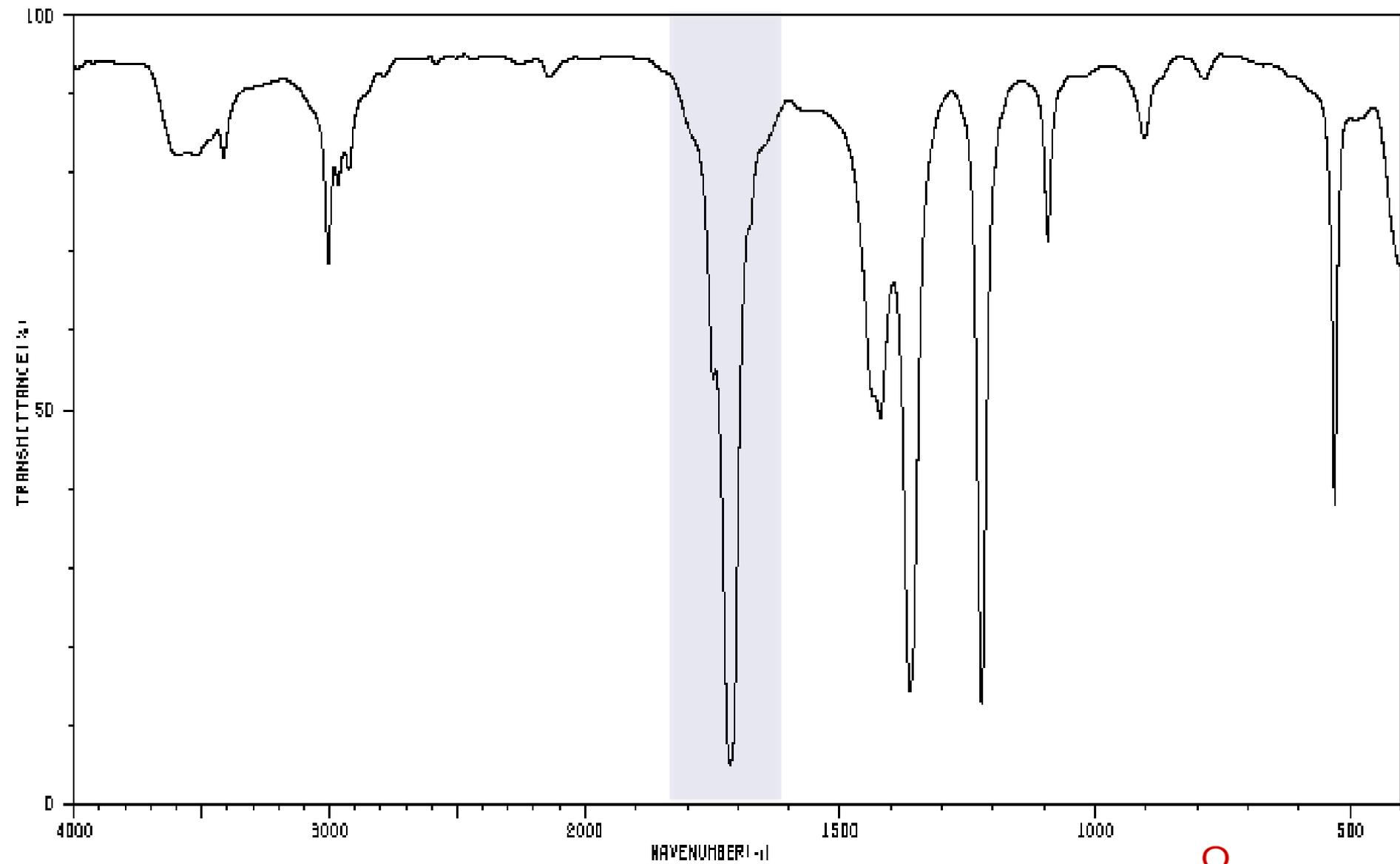


Acid O-H

C=O

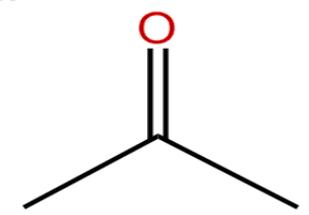
butanoic acid

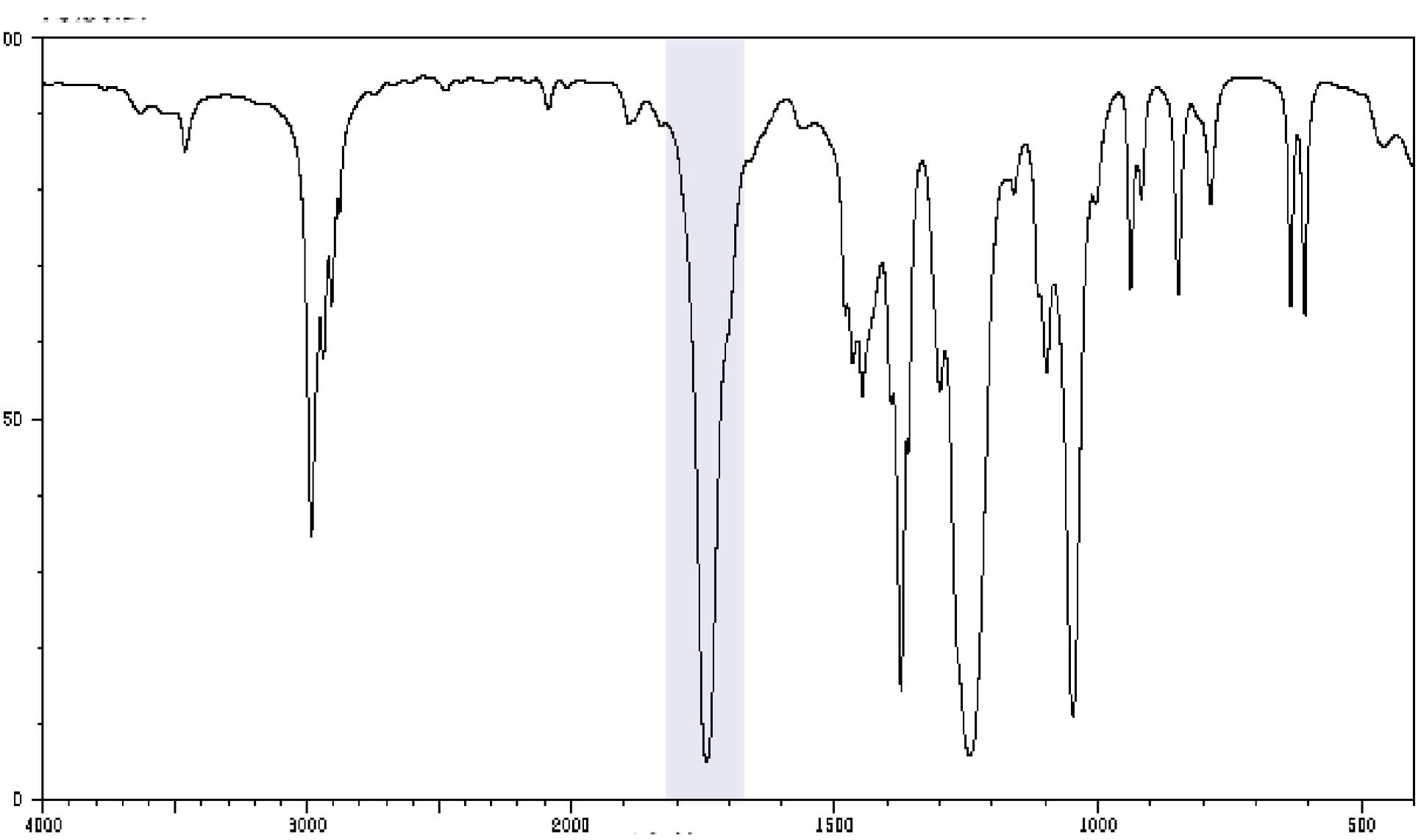




C=O

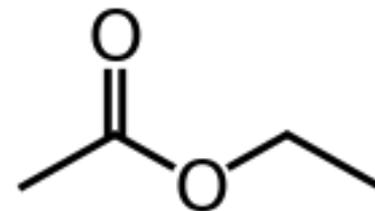
propanone

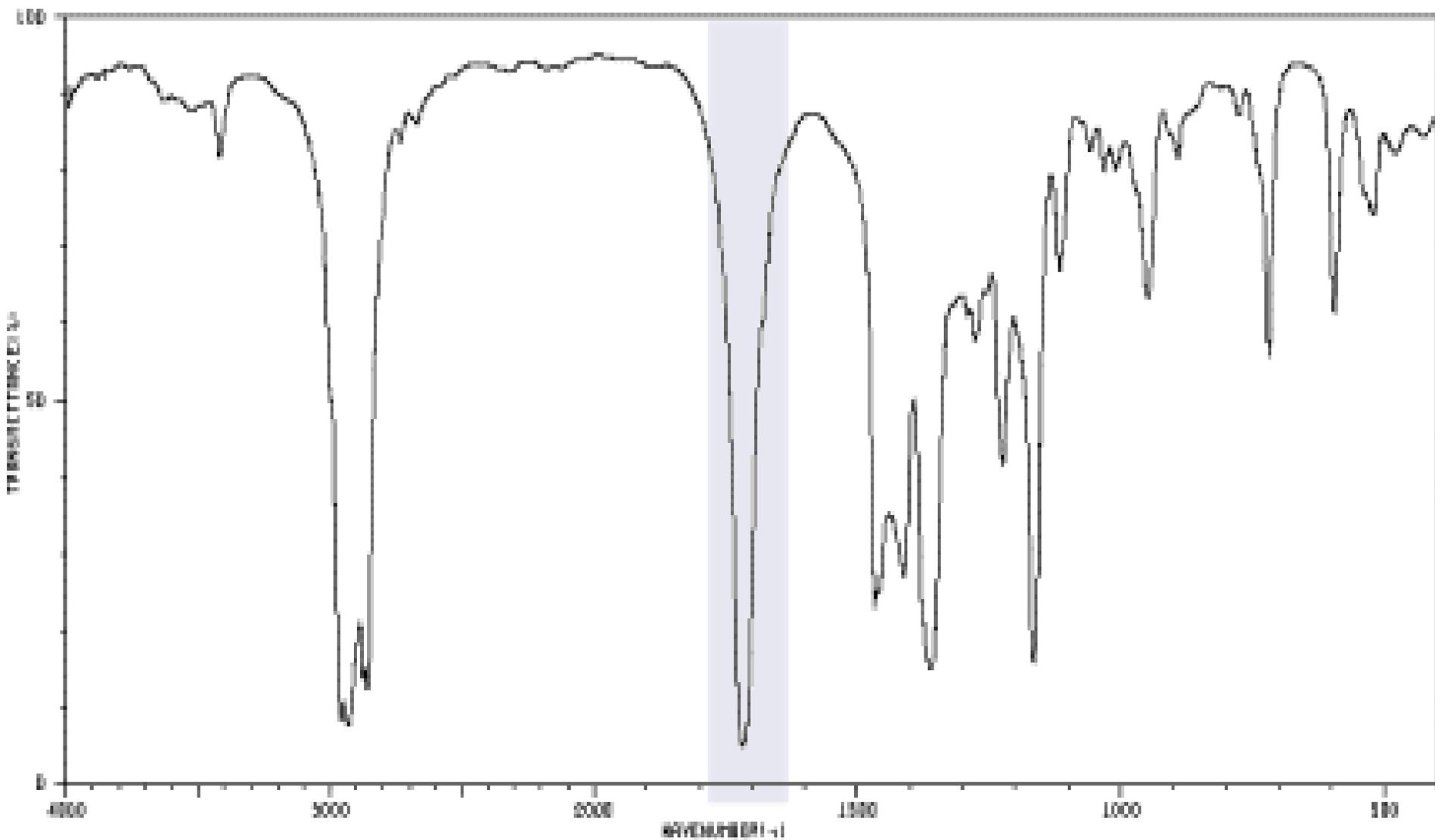




C=O

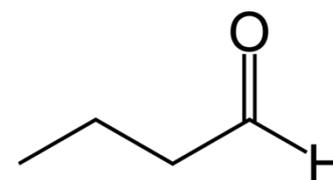
ethyl ethanoate

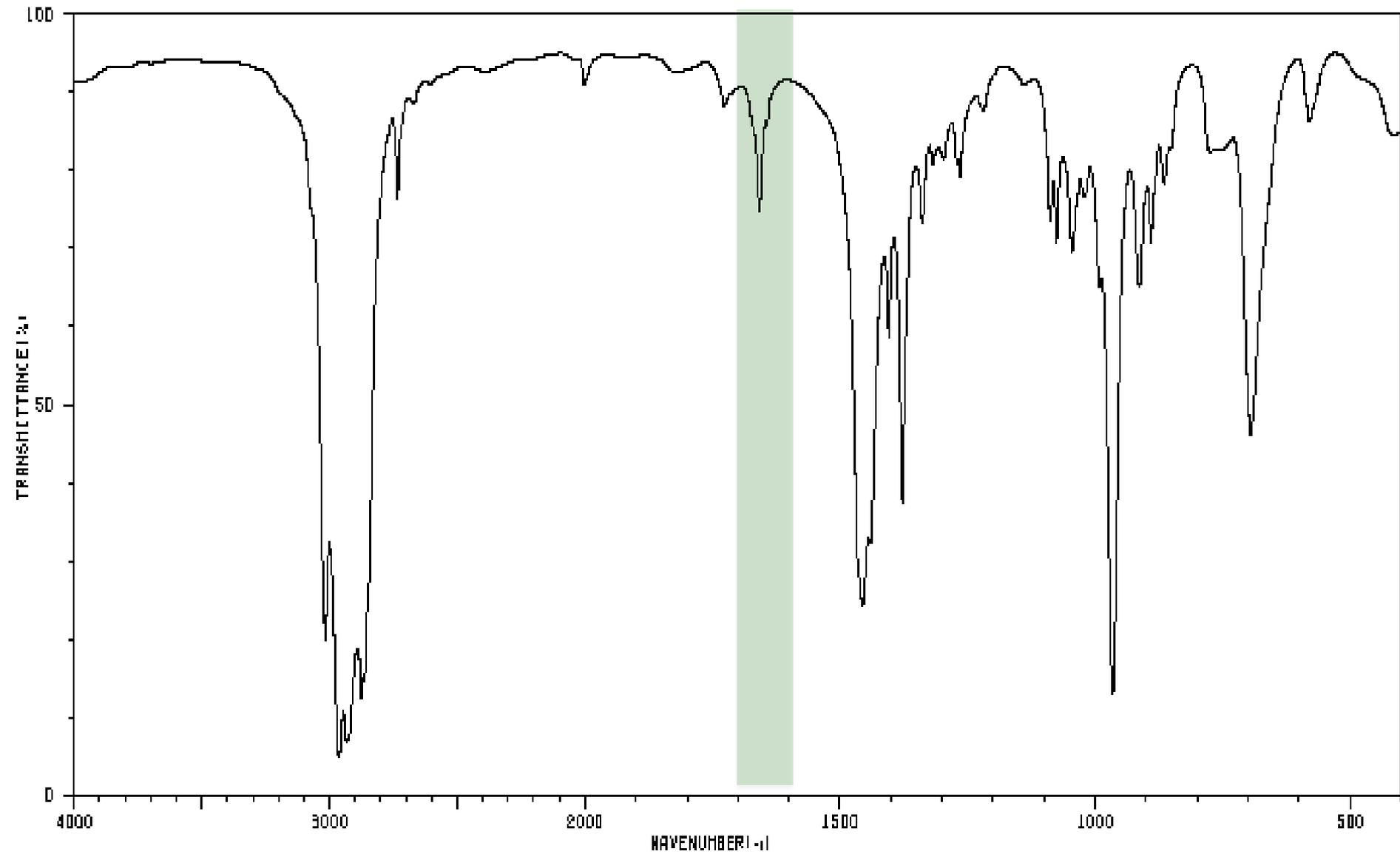




C=O

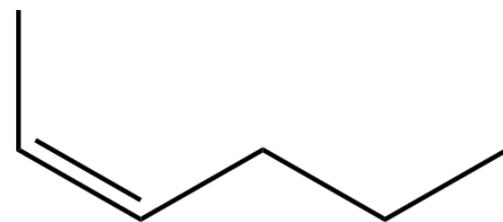
butanal

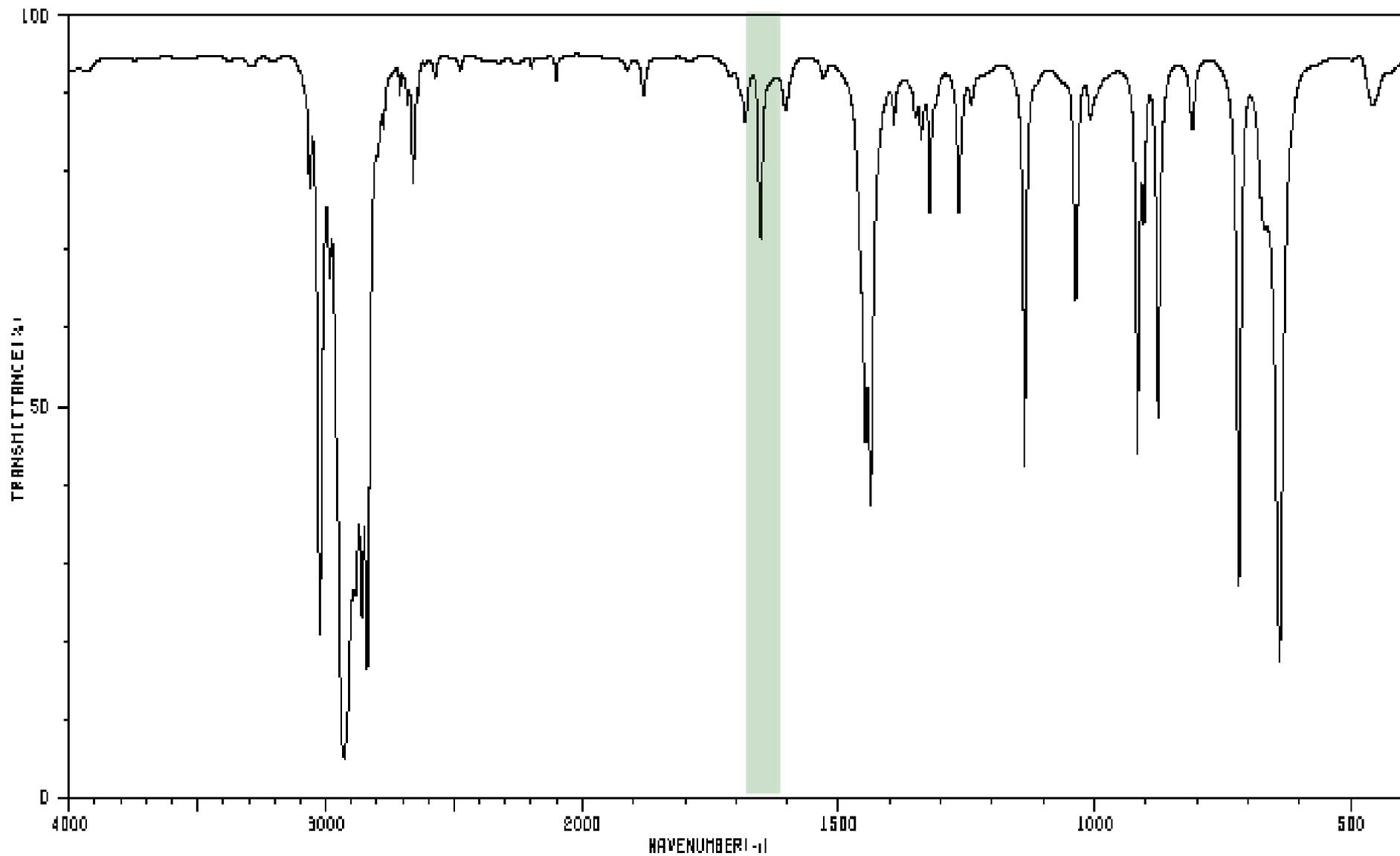




C=C

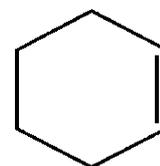
hex-2-ene

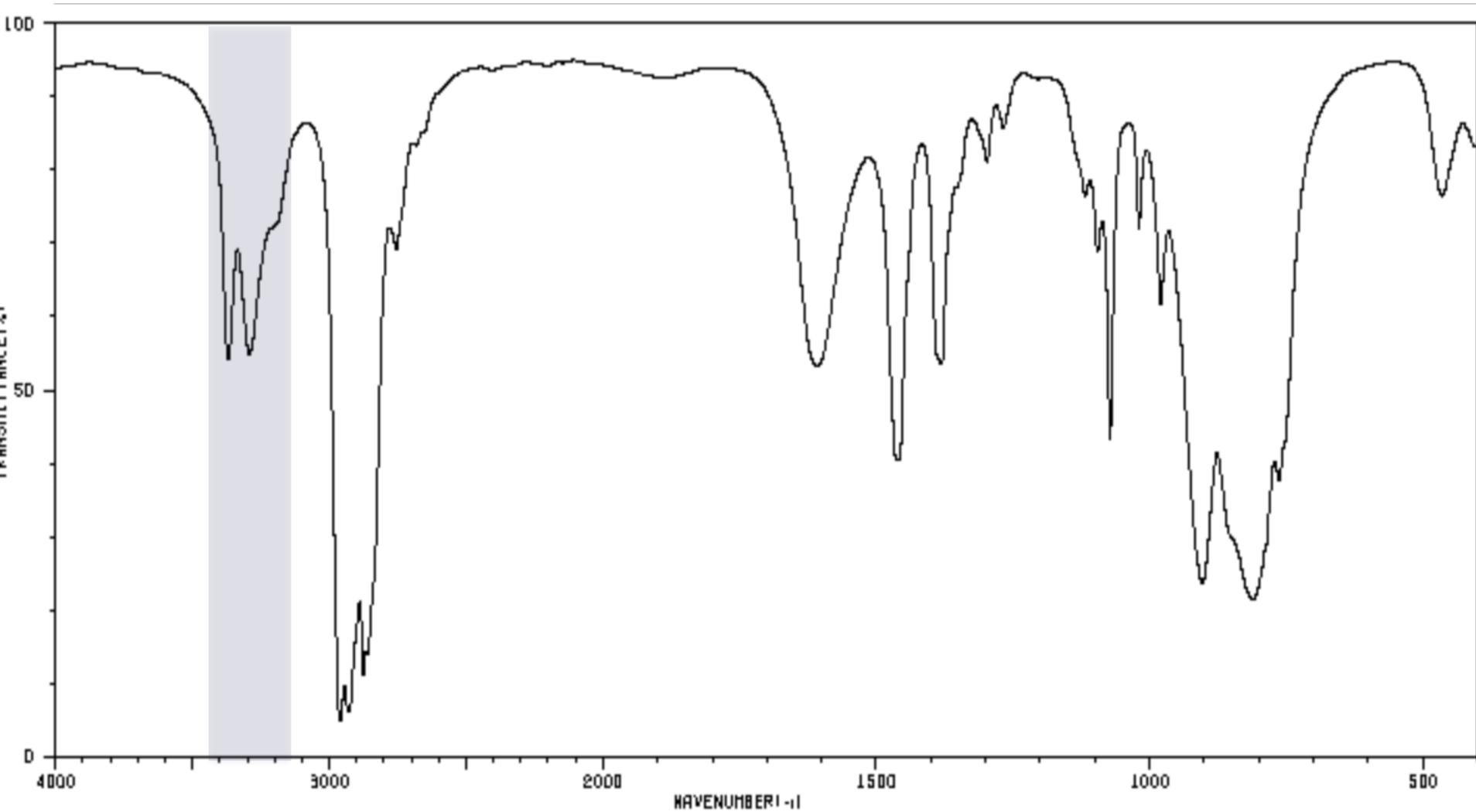




C=C

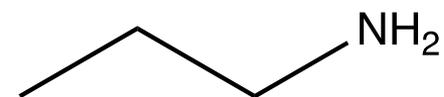
cyclohexene

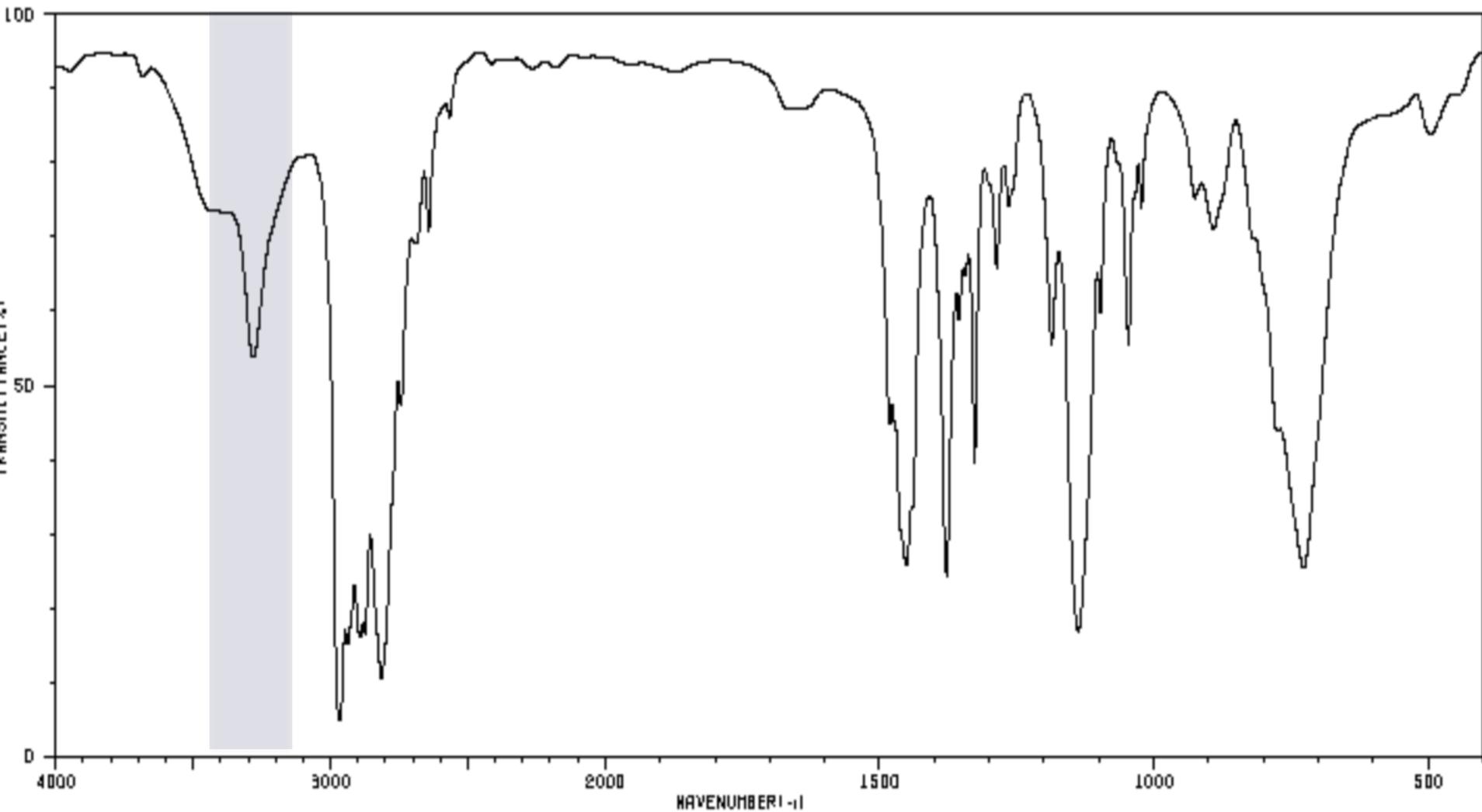




N-H

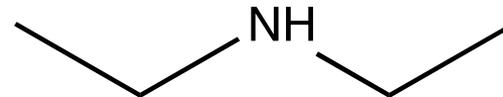
propan-1-amine
(propylamine)

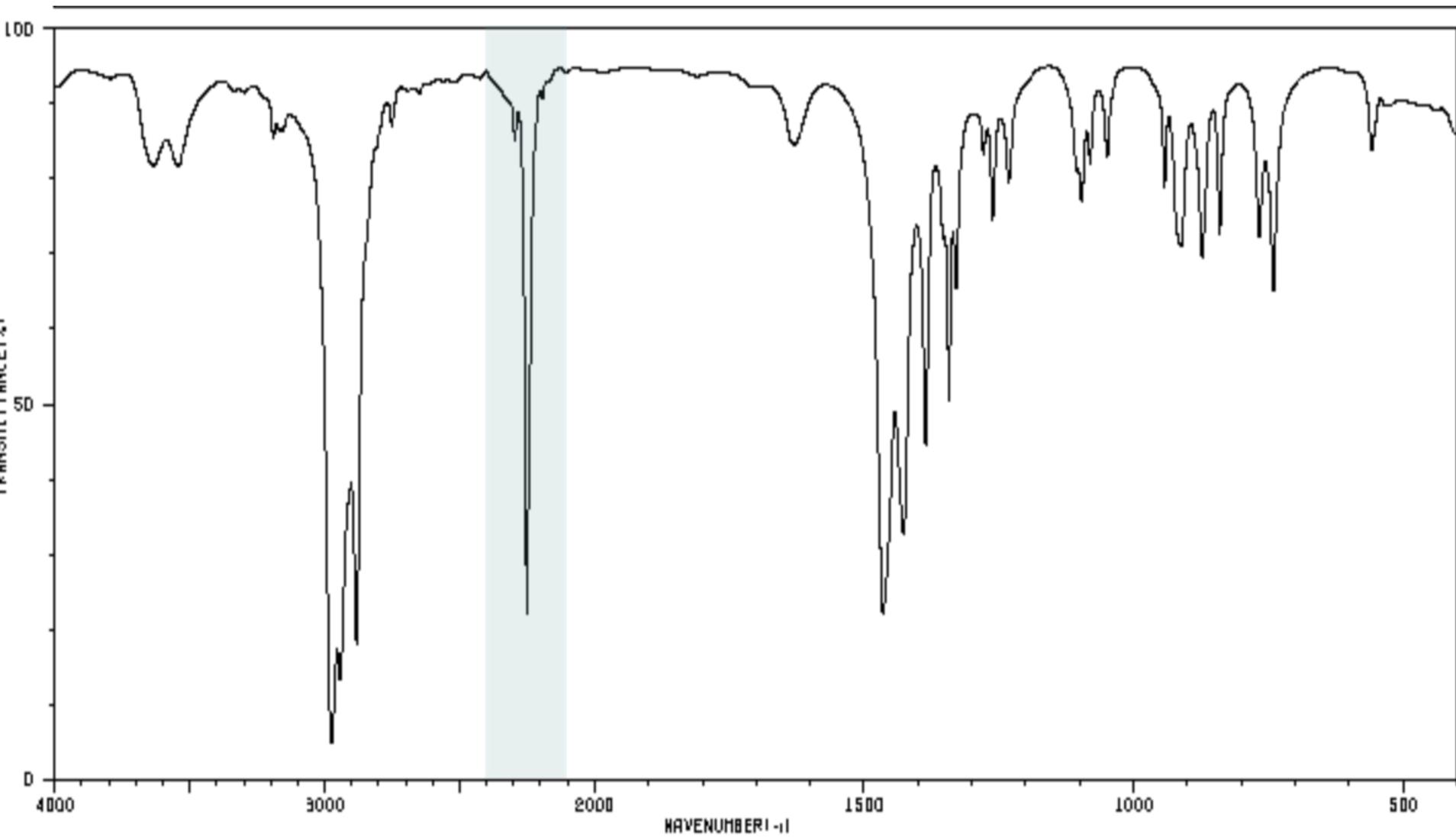




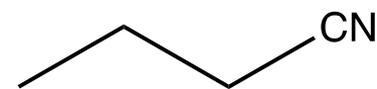
N-H

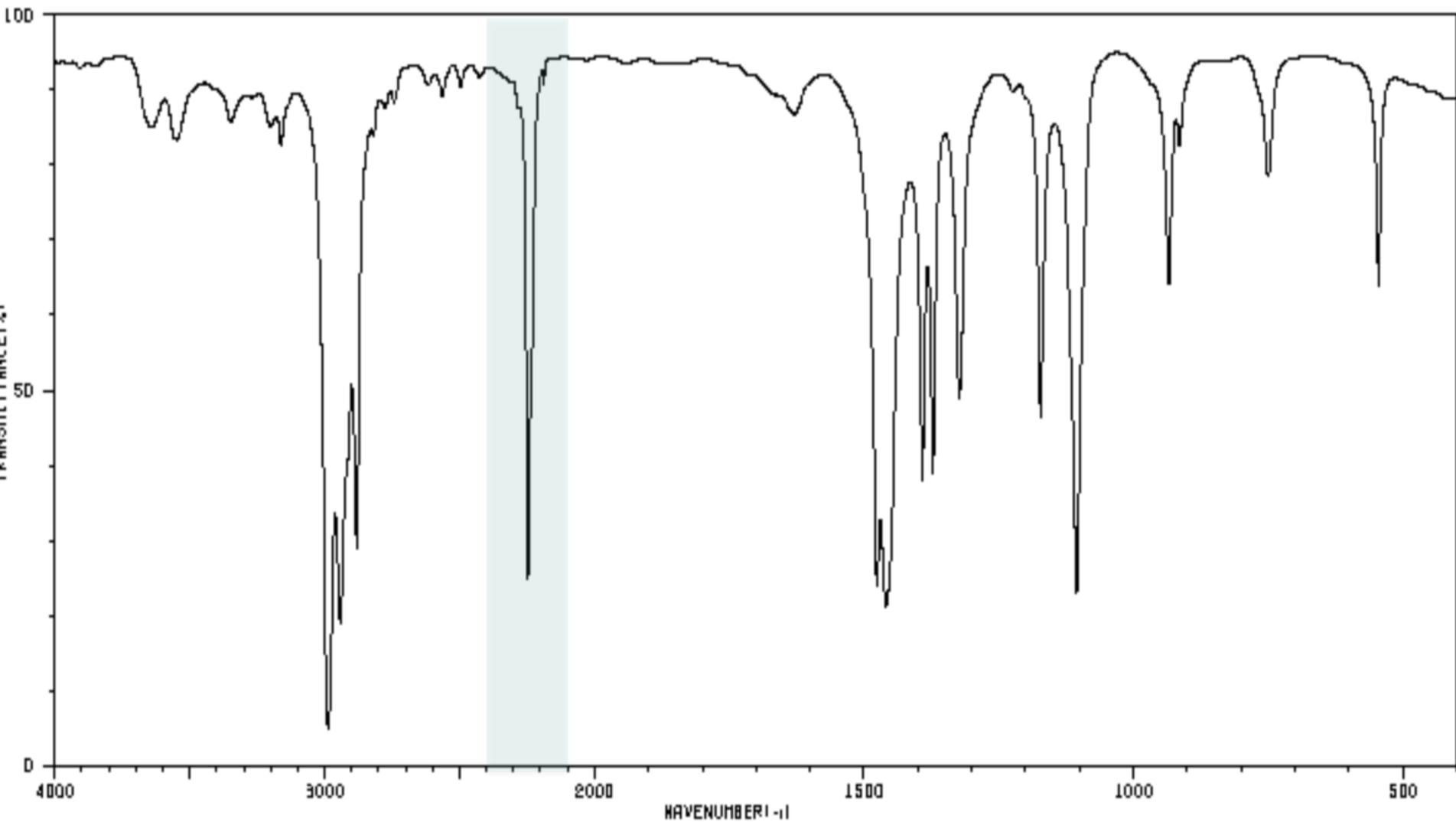
N-ethylethanamine
(diethylamine)





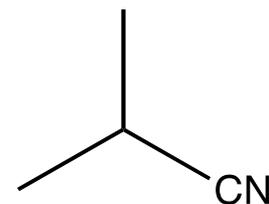
butanenitrile



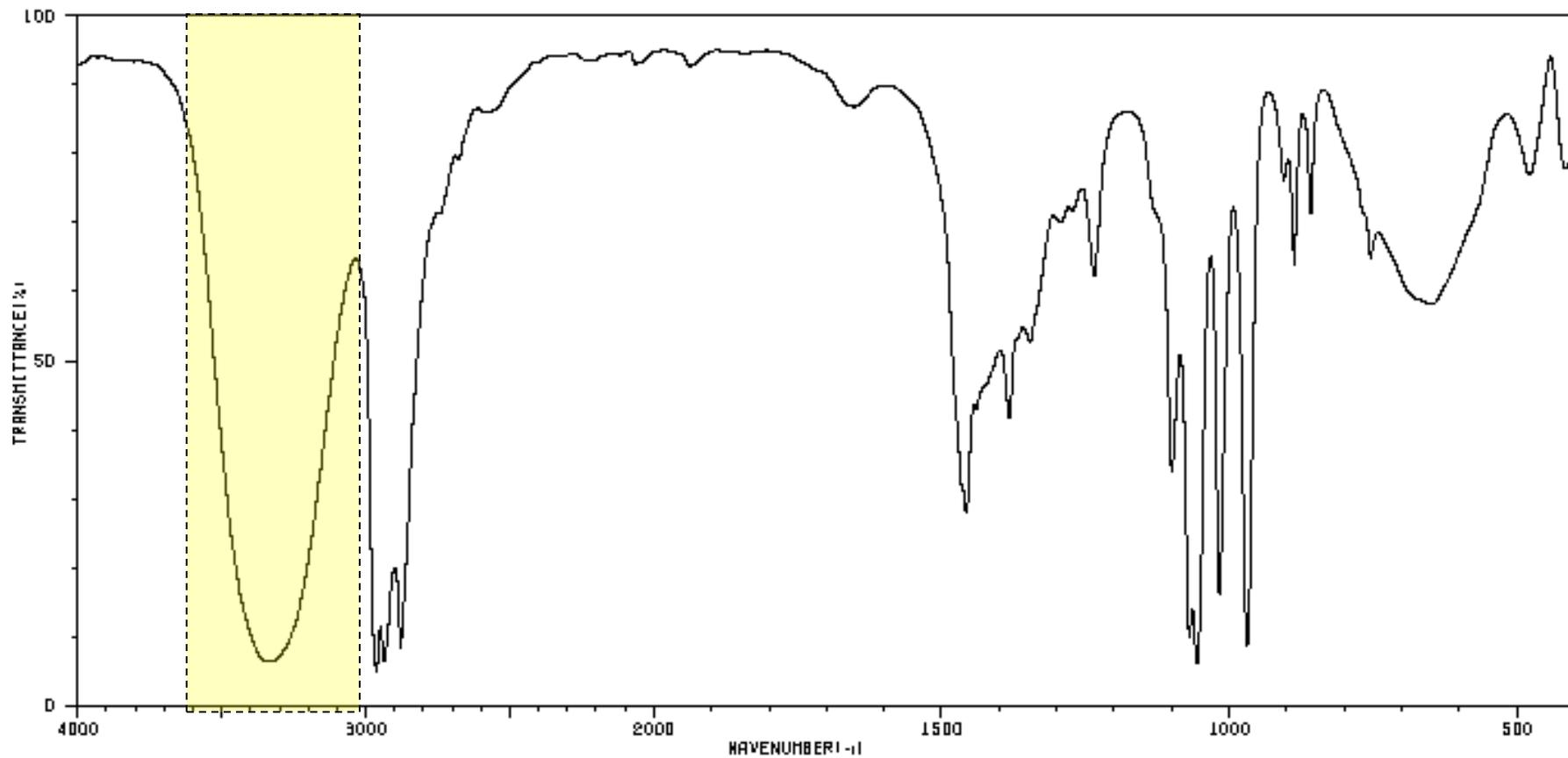


C≡N

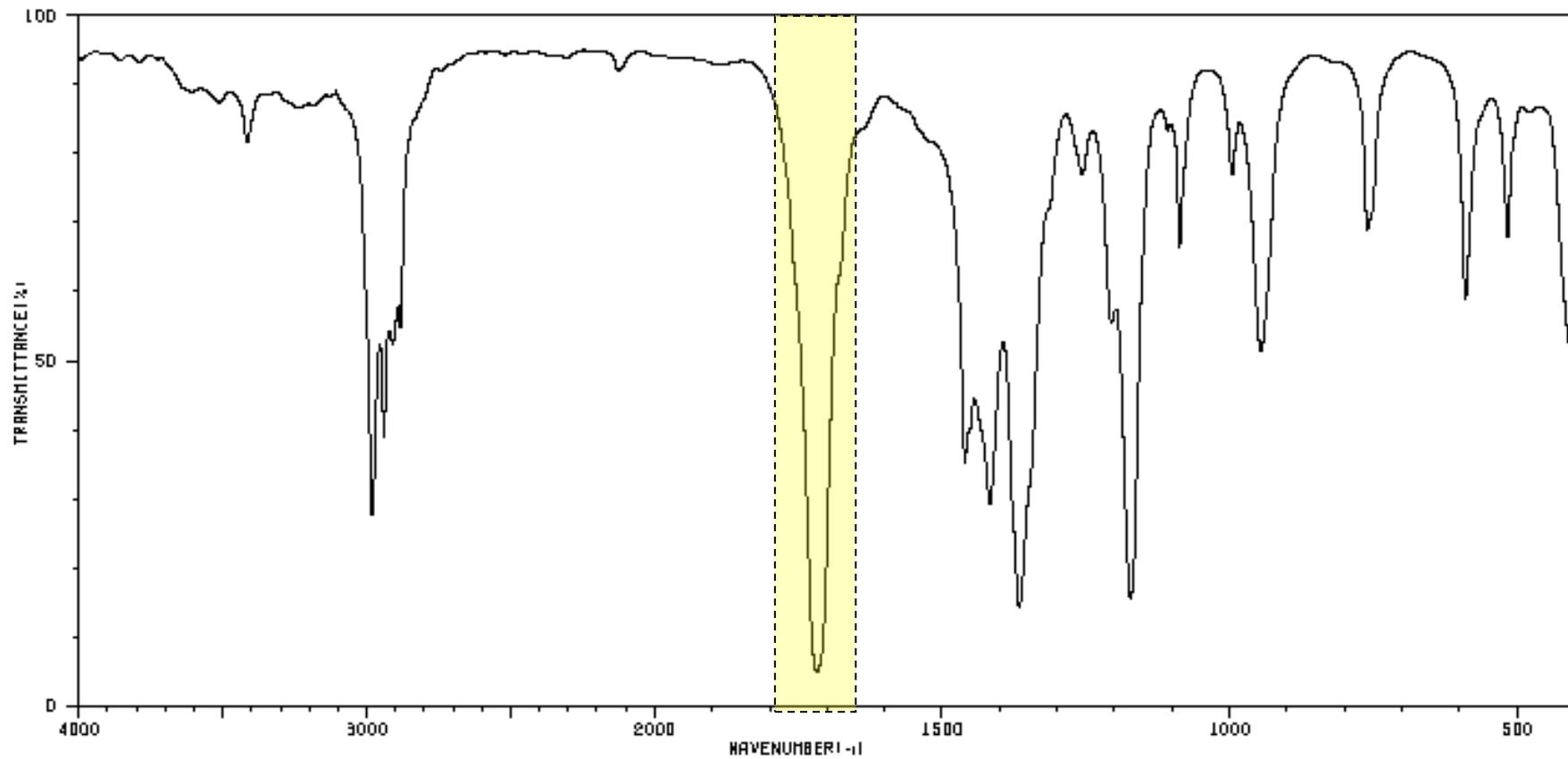
2-methylpropanenitrile

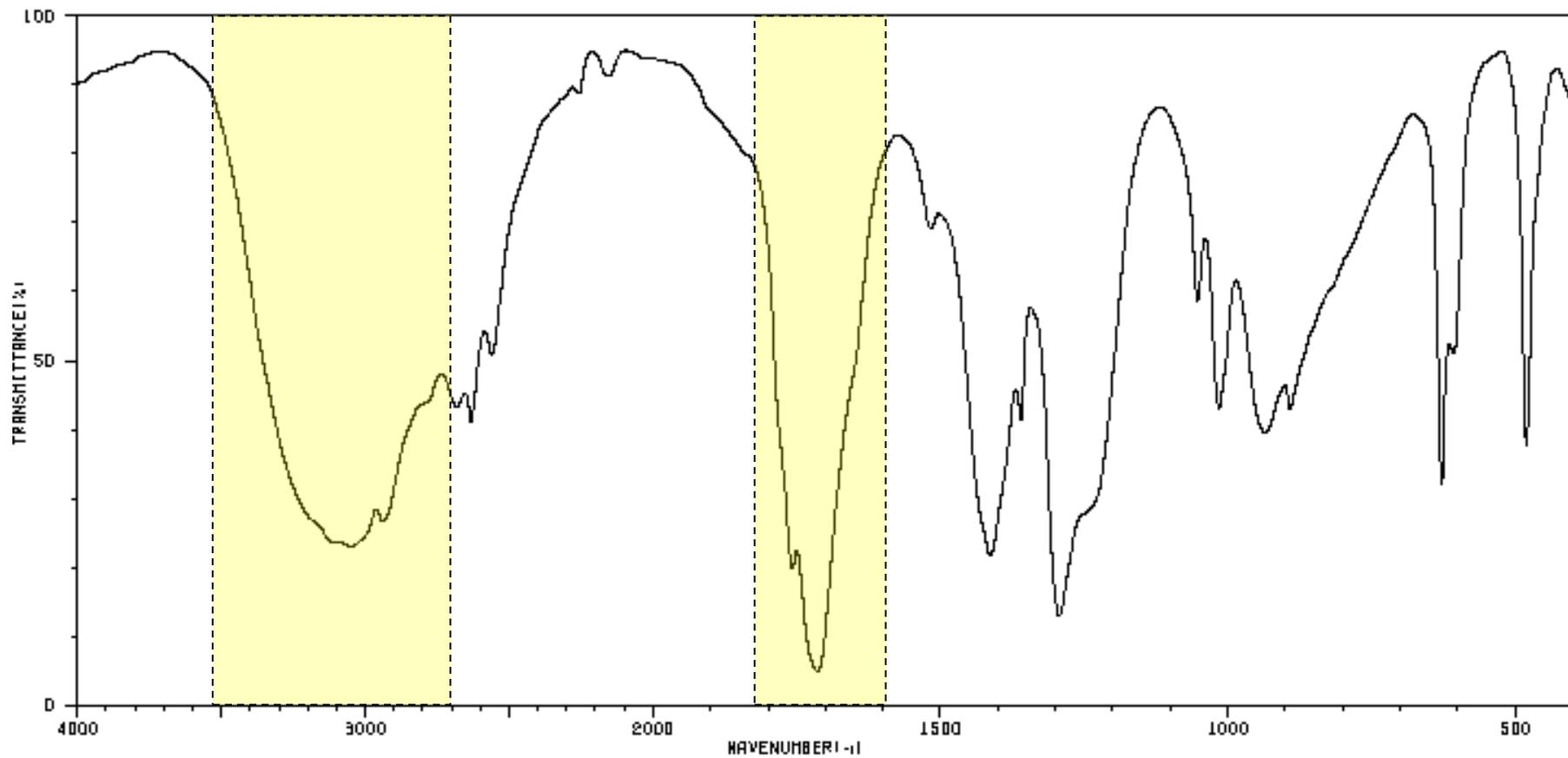


Identify the Functional Groups

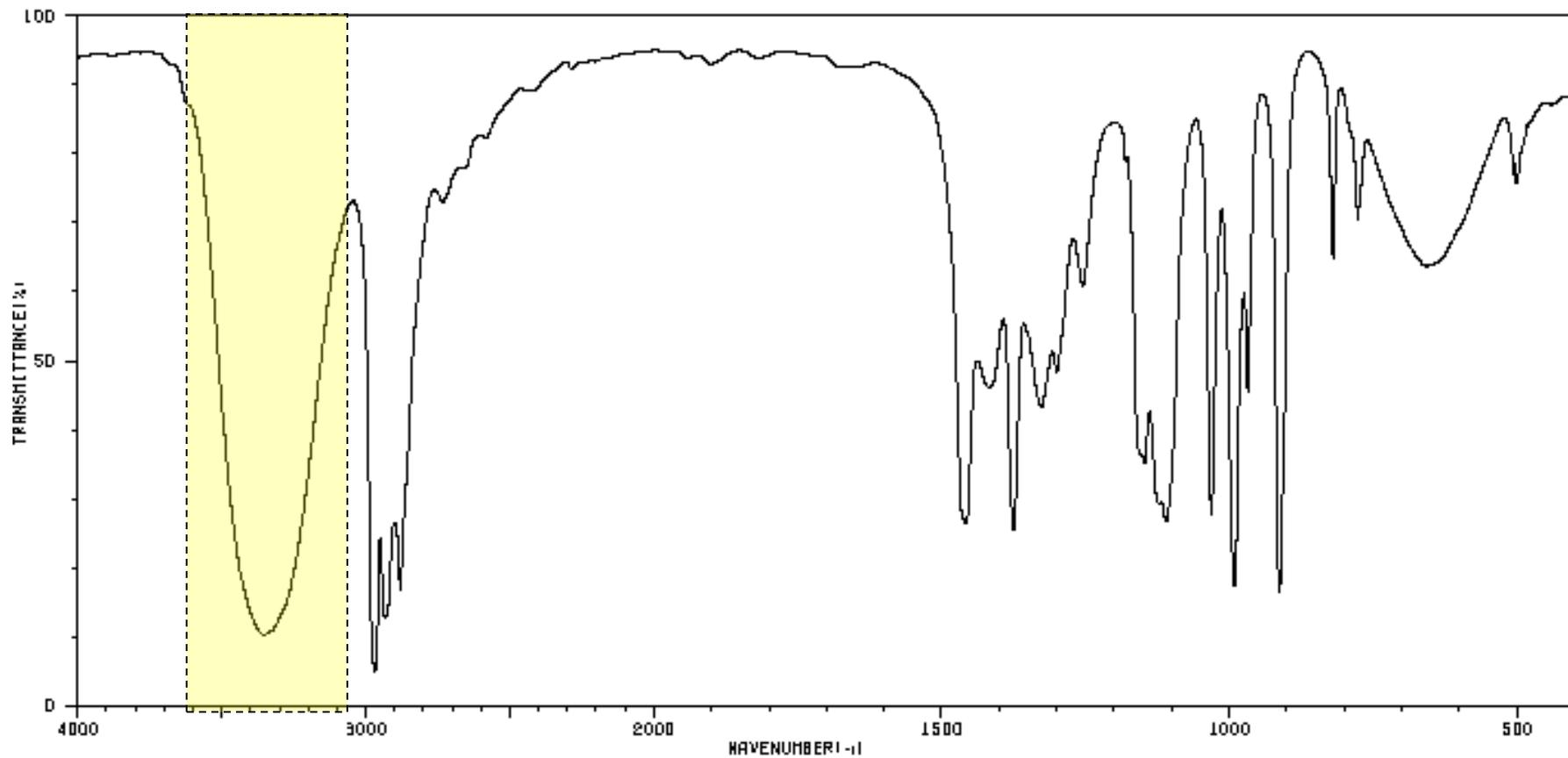


Alcohol O-H

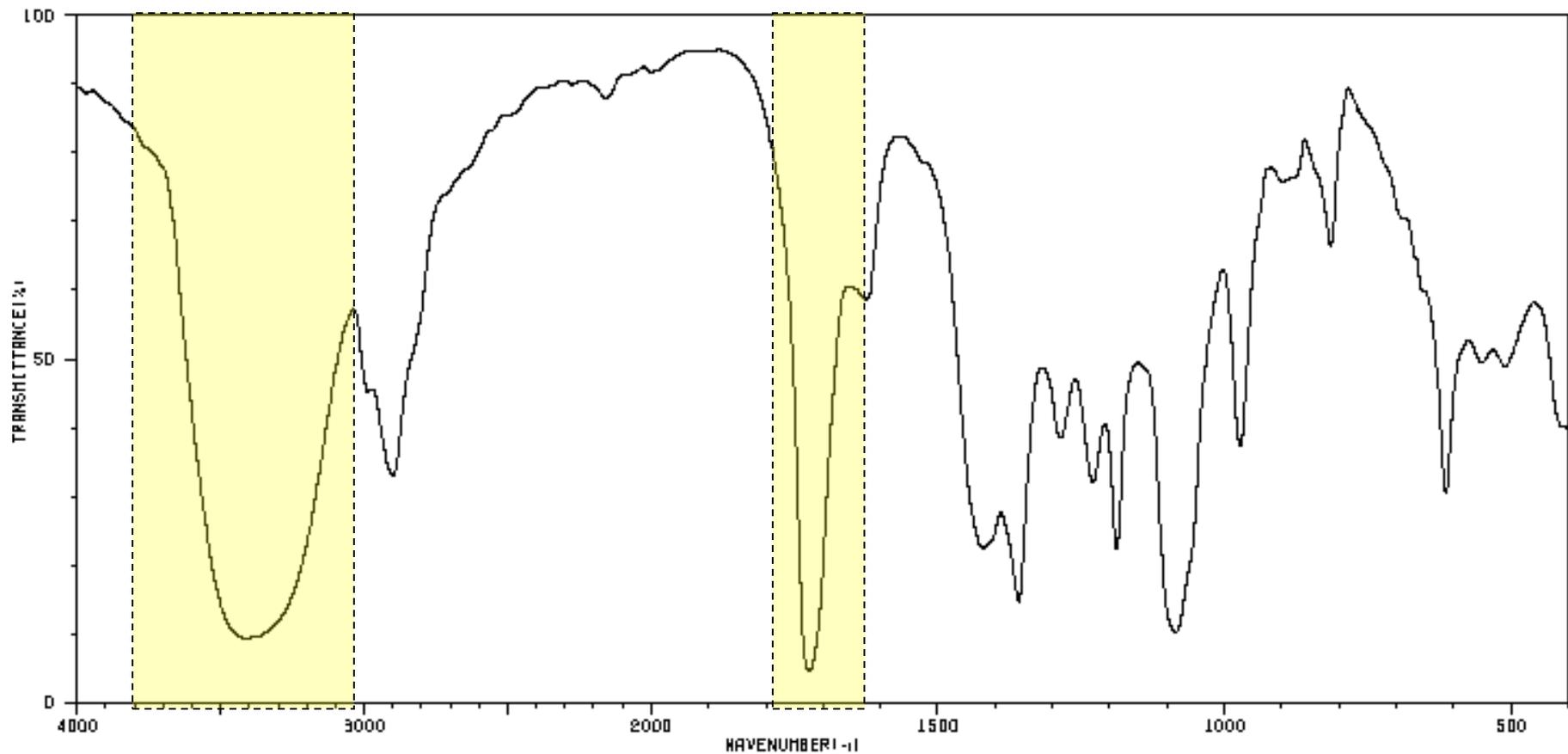




C=O
acid O-H

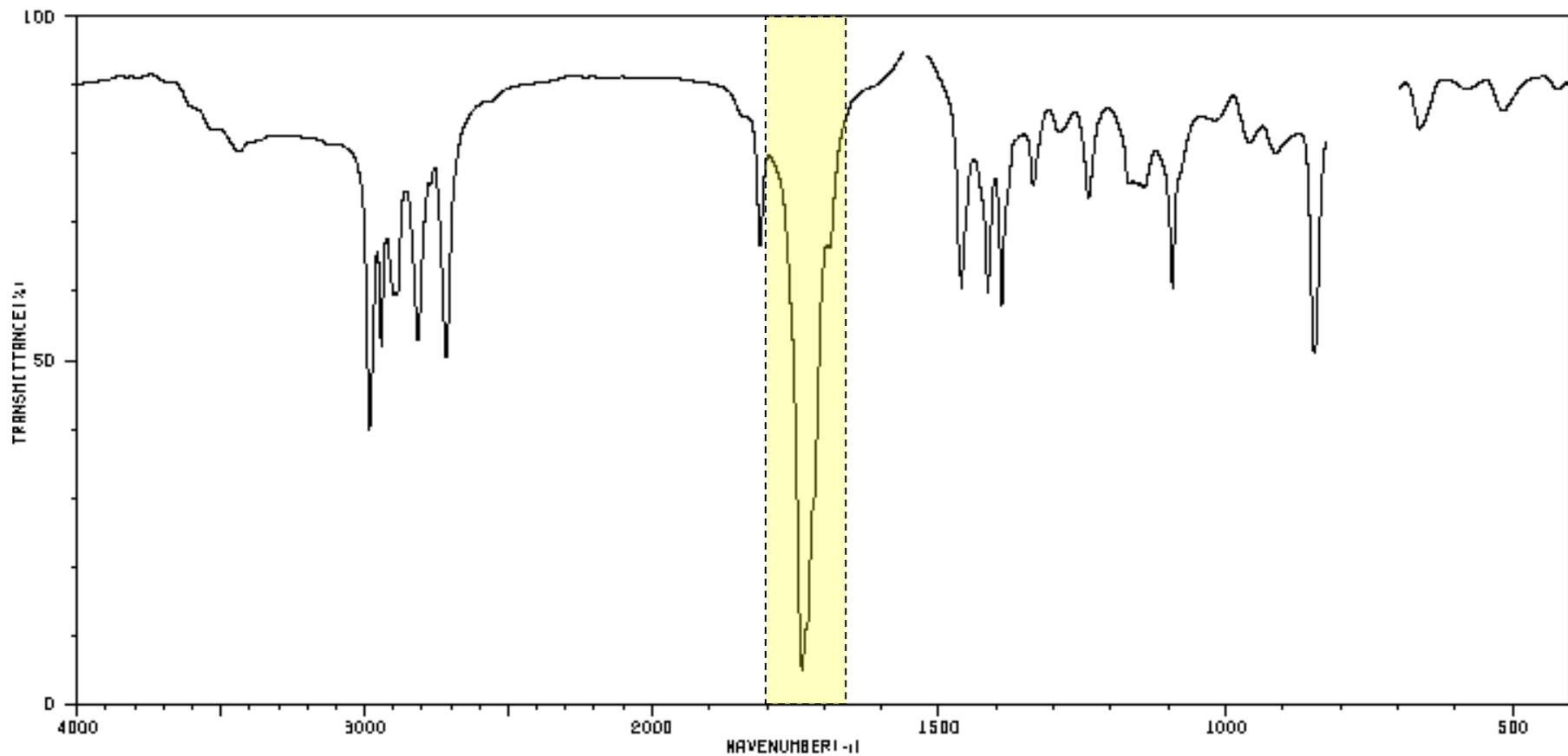


Alcohol O-H

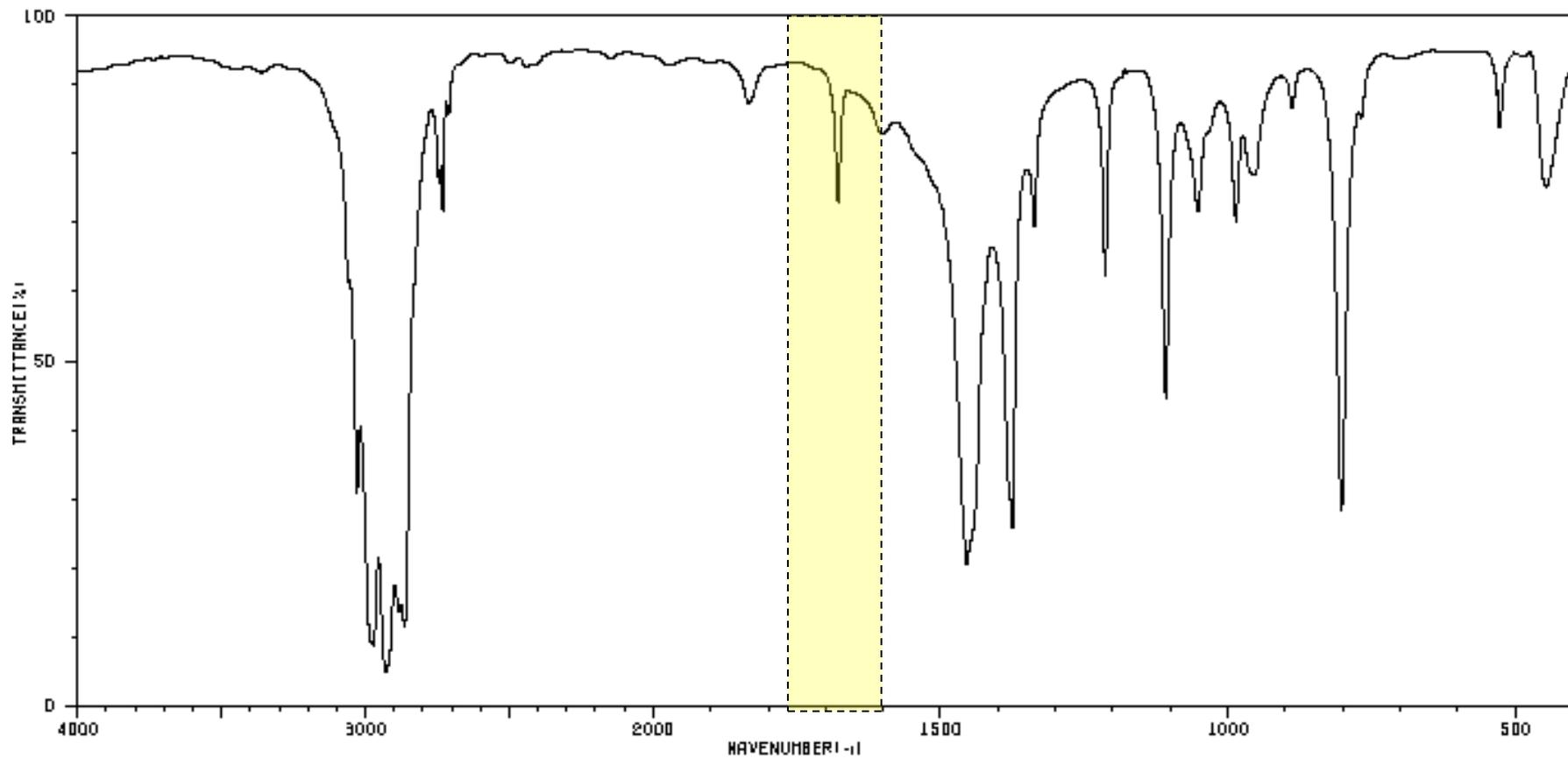


C=O

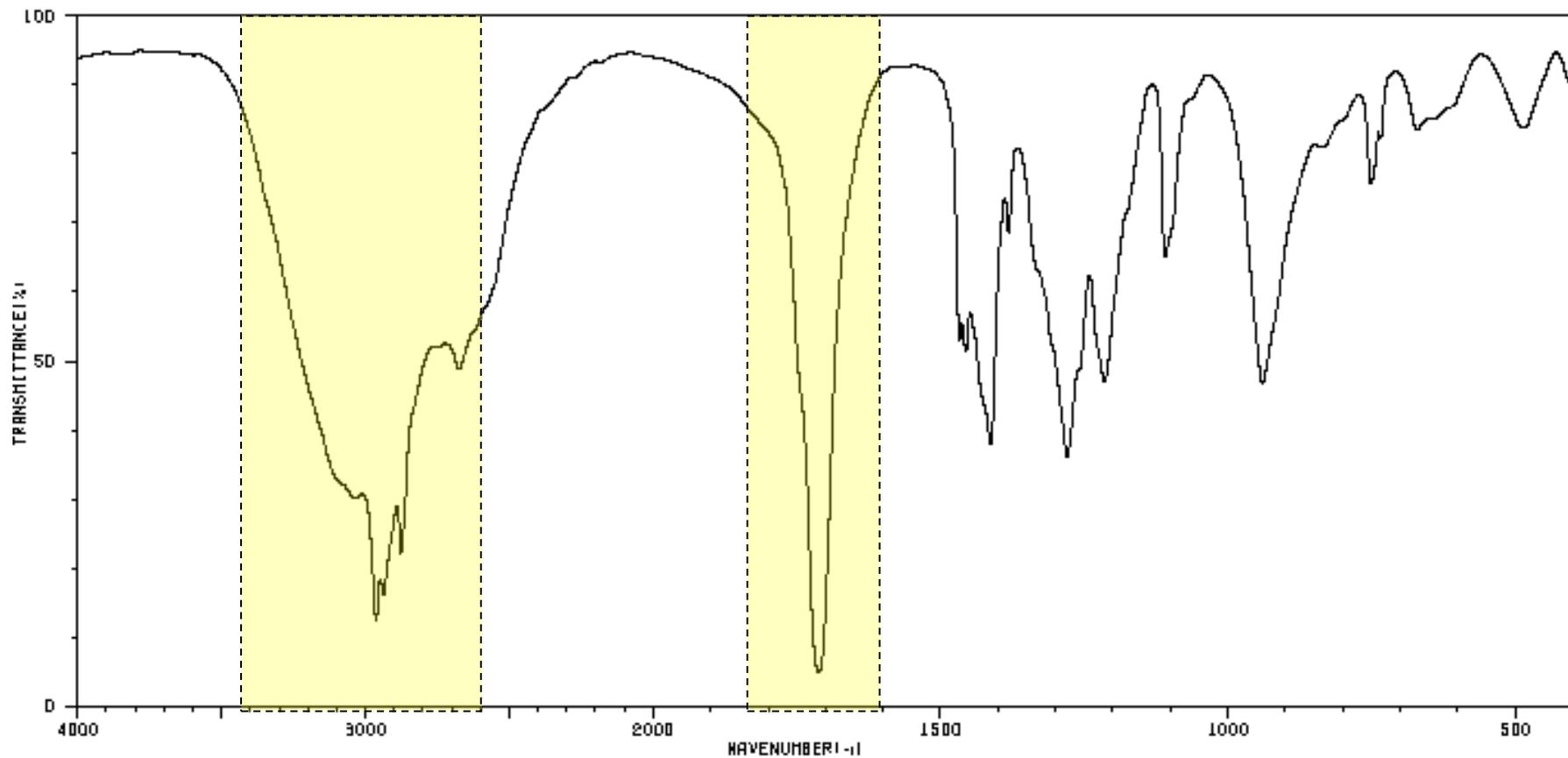
alcohol O-H



C=O

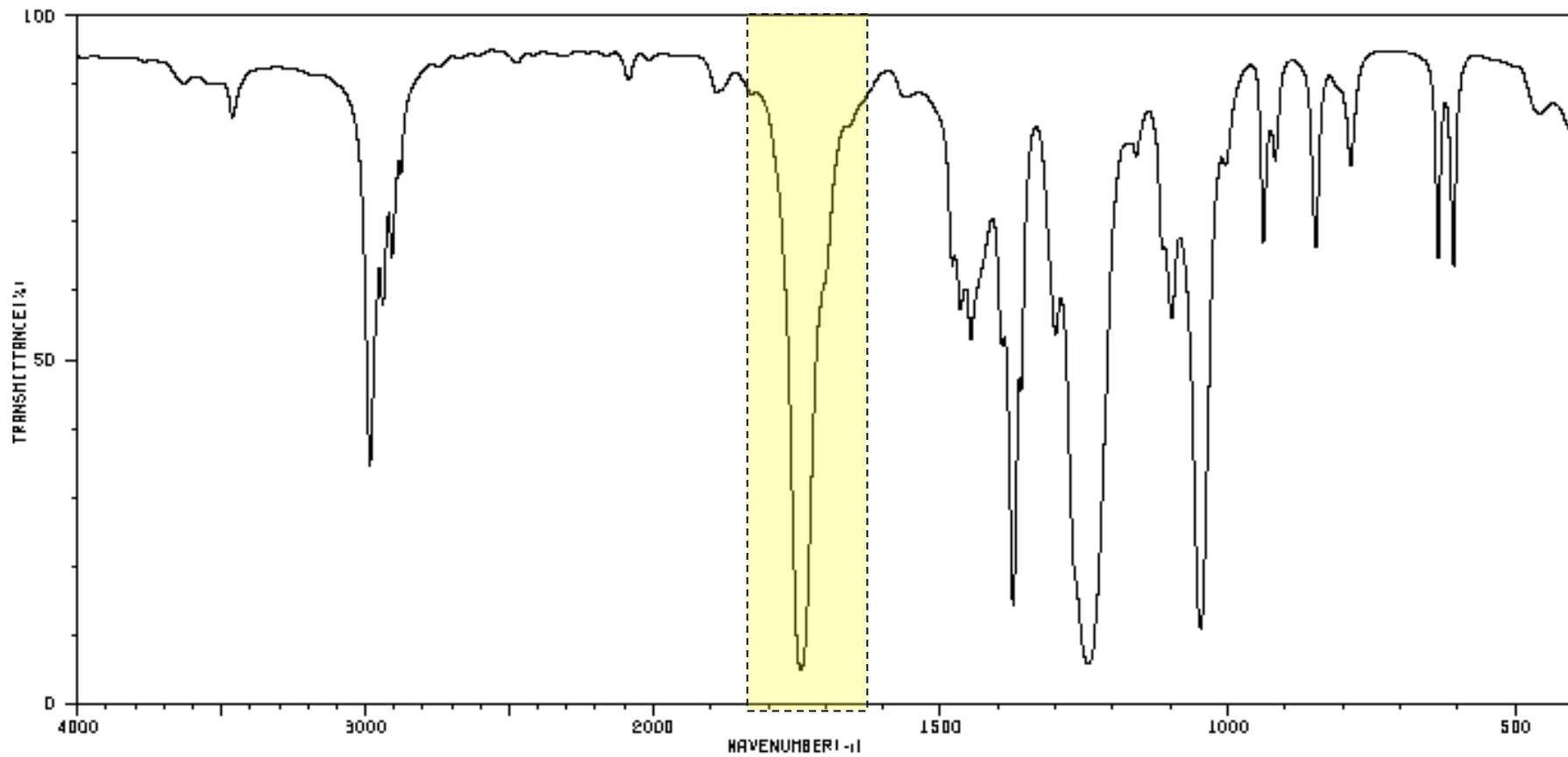


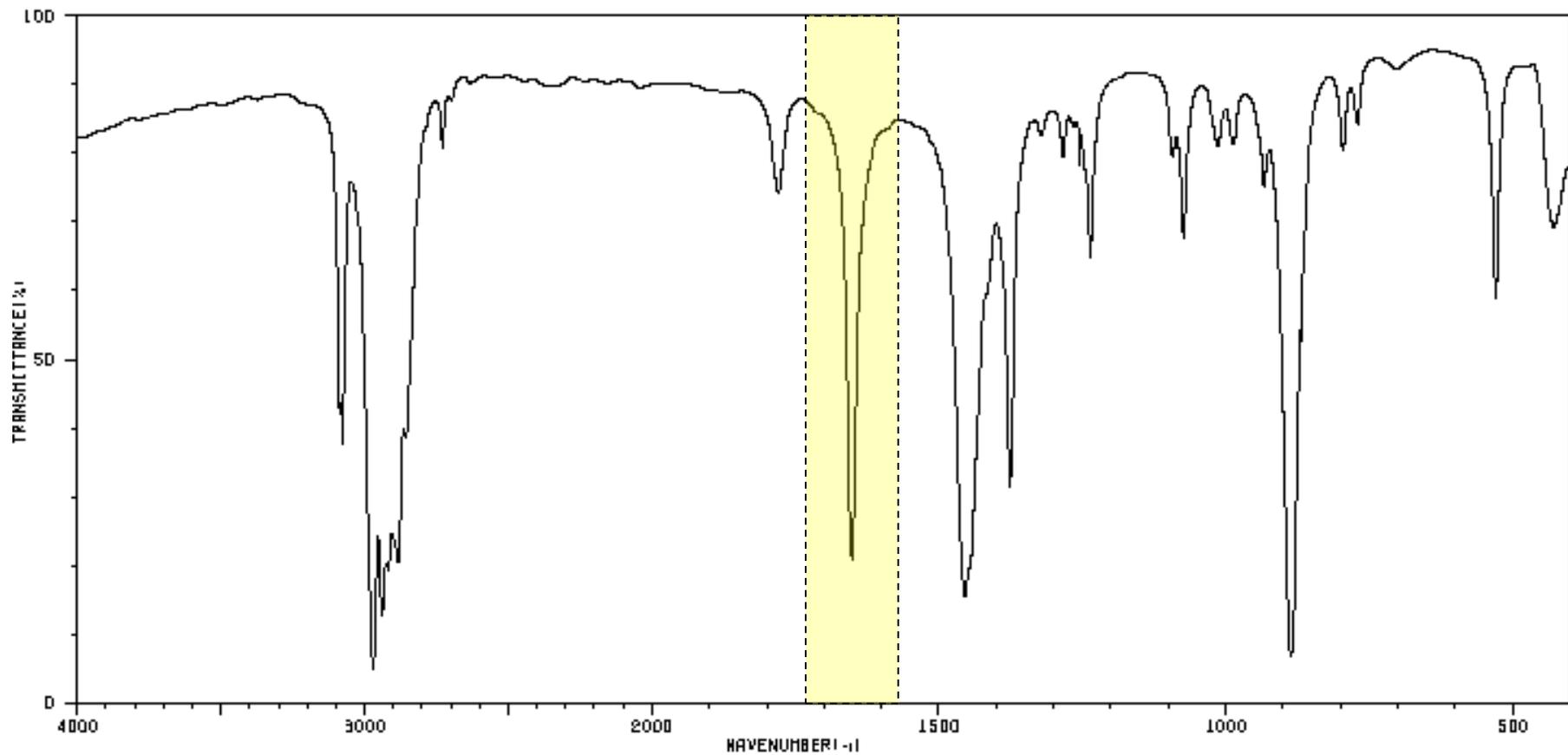
C=C



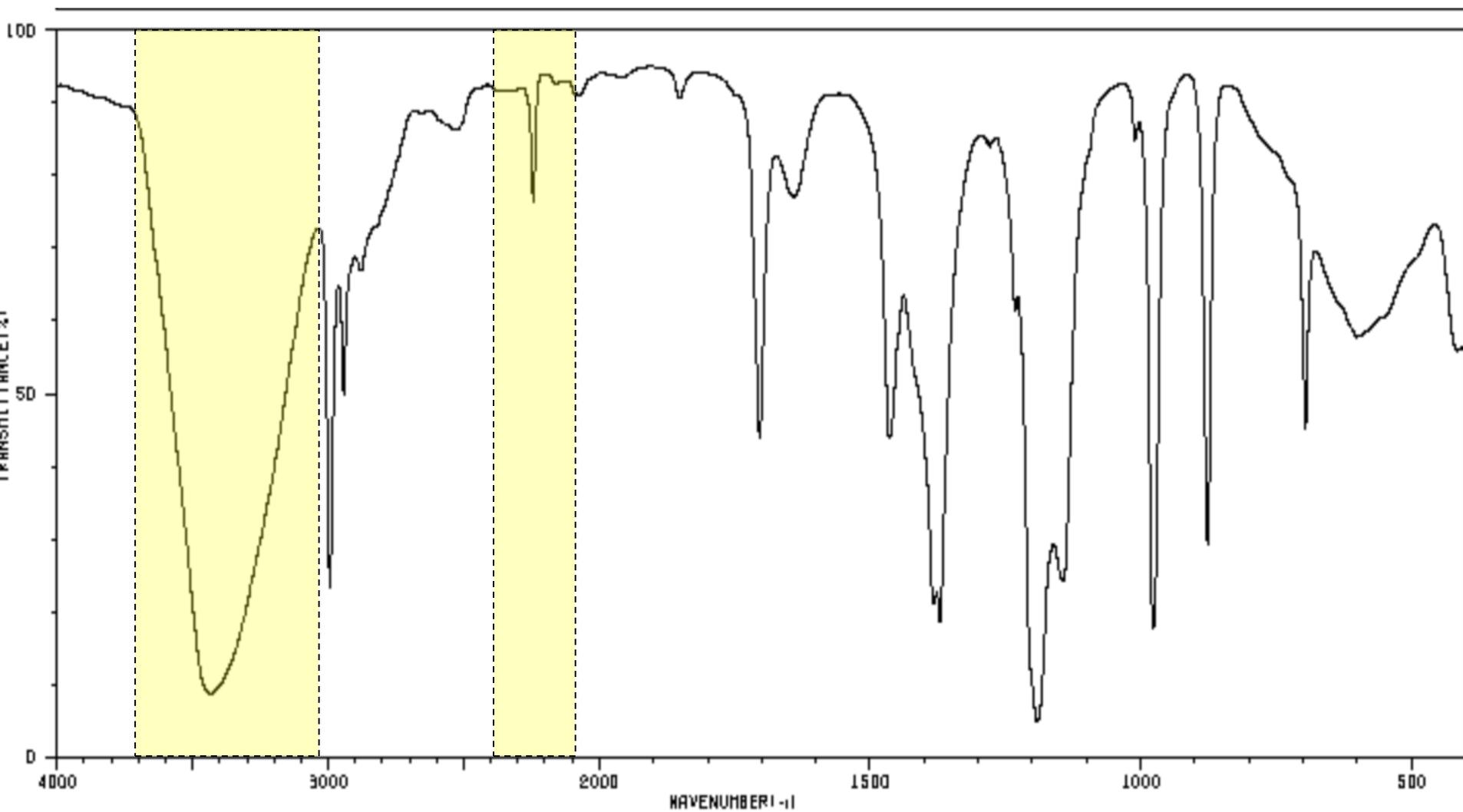
C=O

acid O-H





C=C



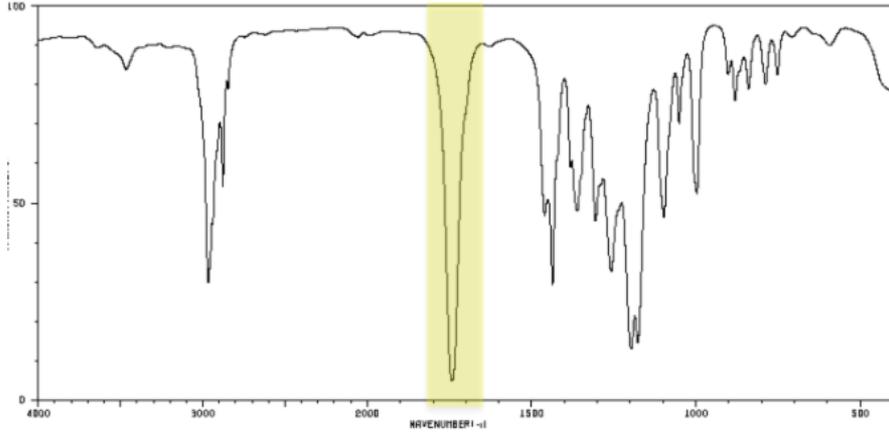
$\text{C}\equiv\text{N}$

alcohol O-H

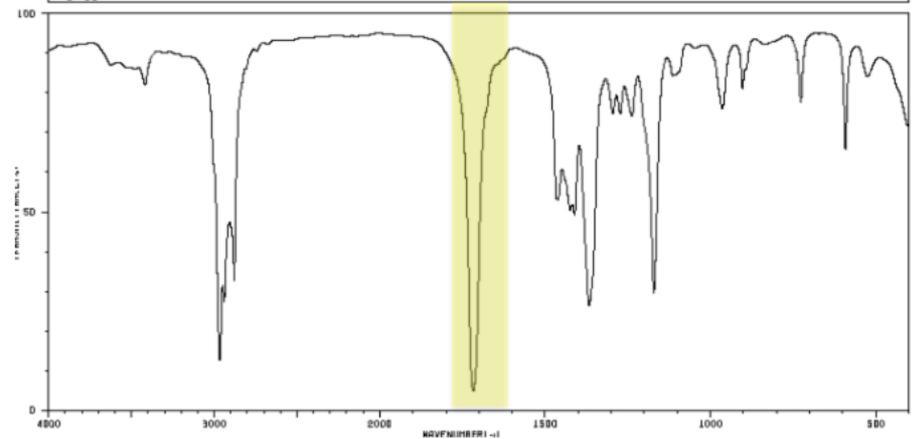
IR Problems A

Which of these compounds contain a C=O bond?

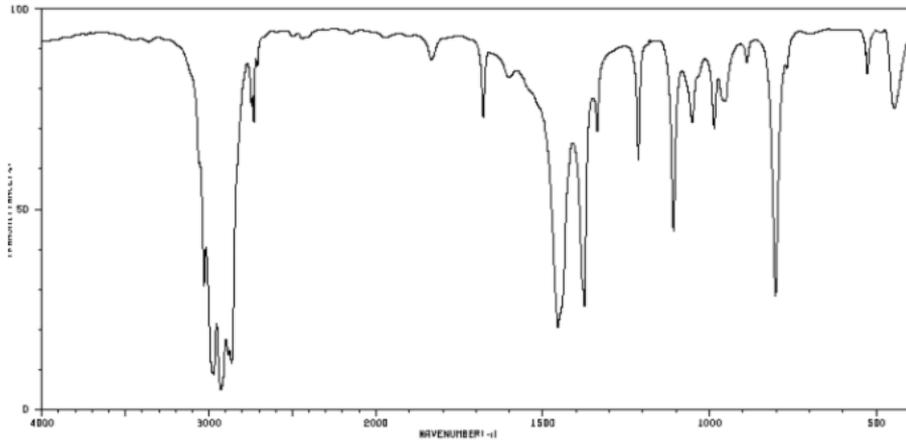
A1



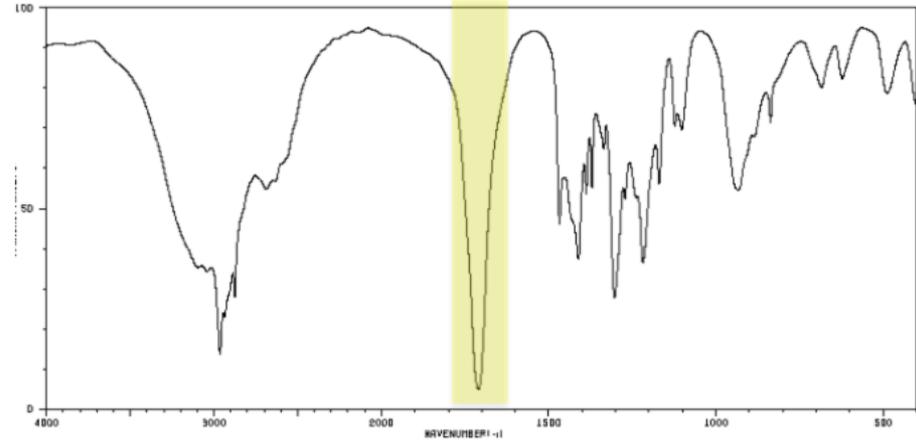
A2



A3

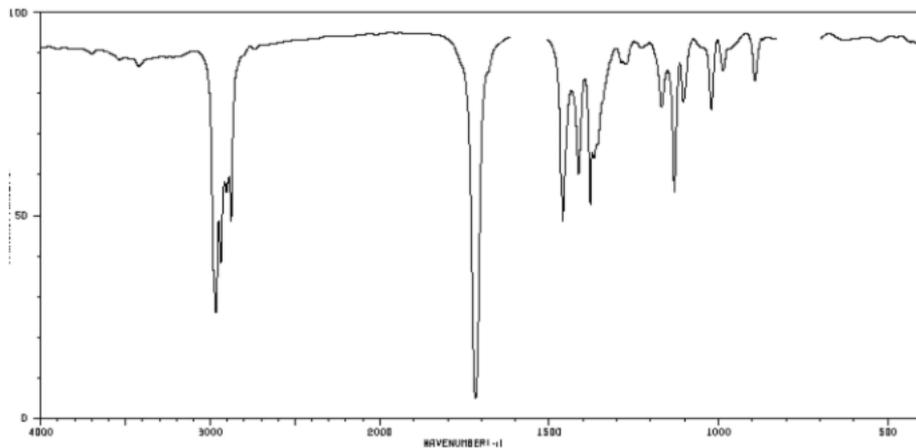


A4

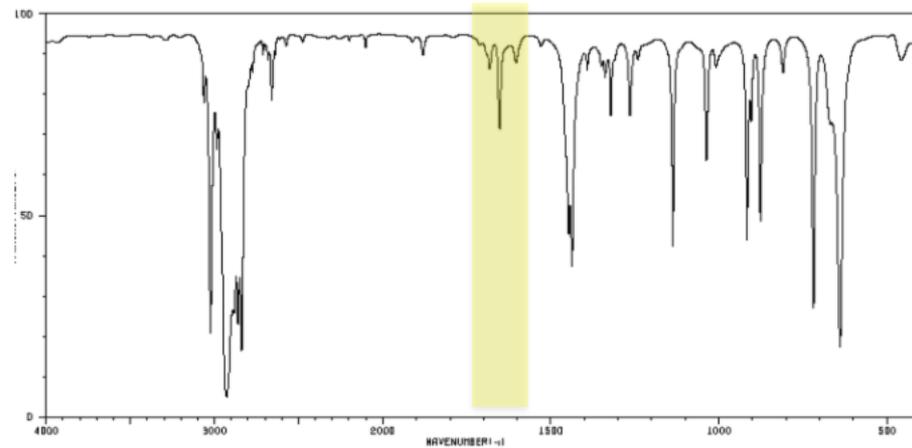


Which of these compounds contain a C=C bond?

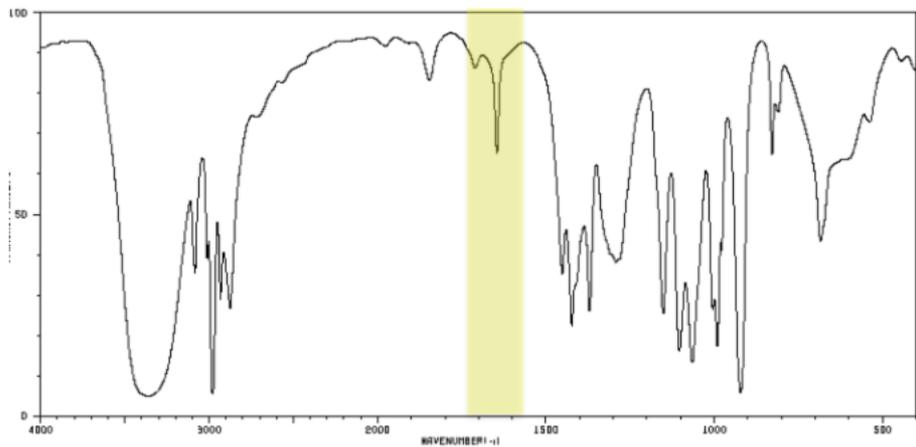
B1



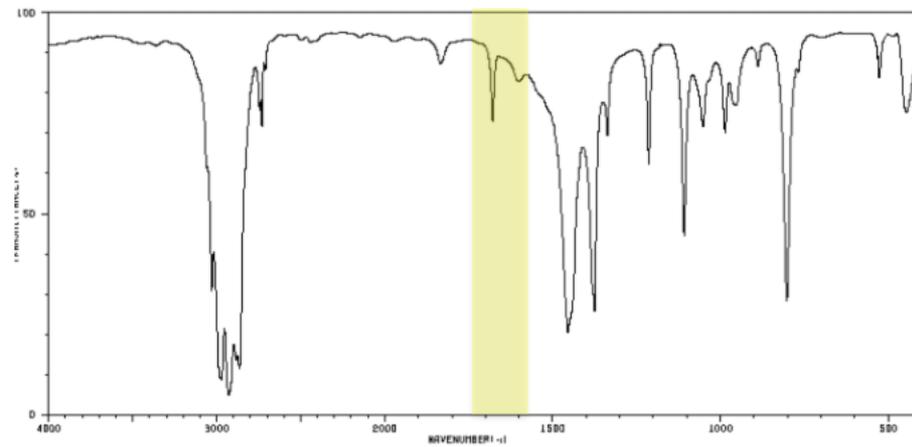
B2



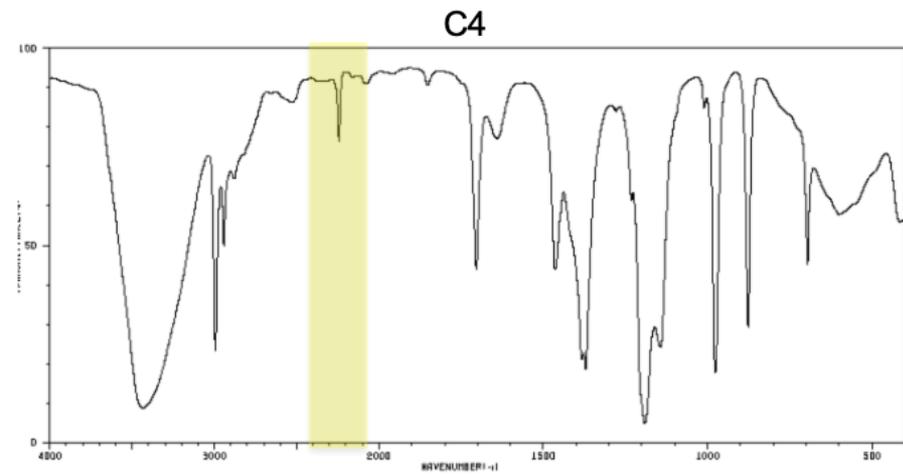
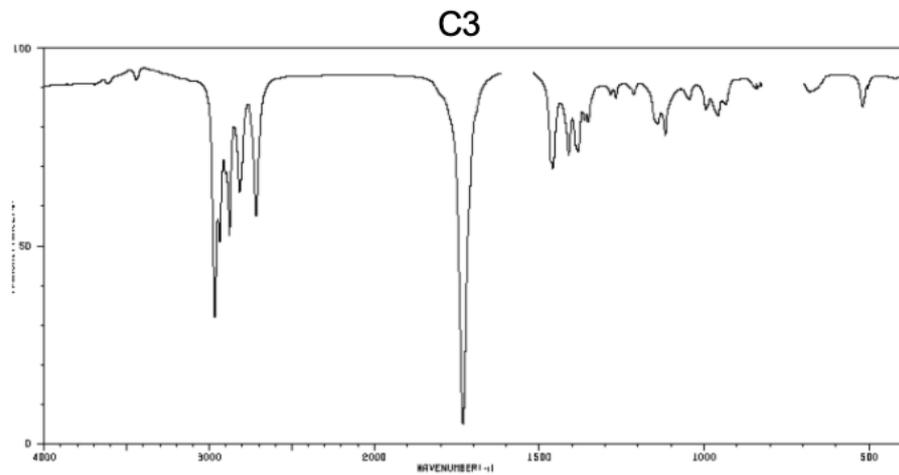
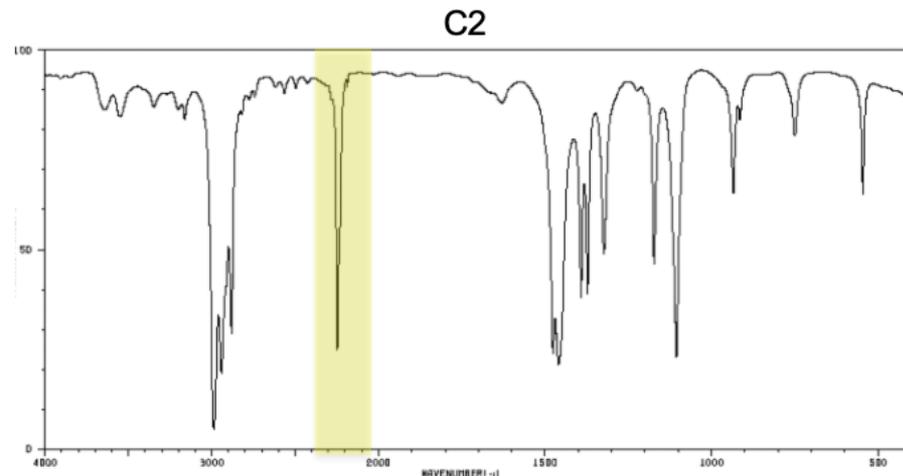
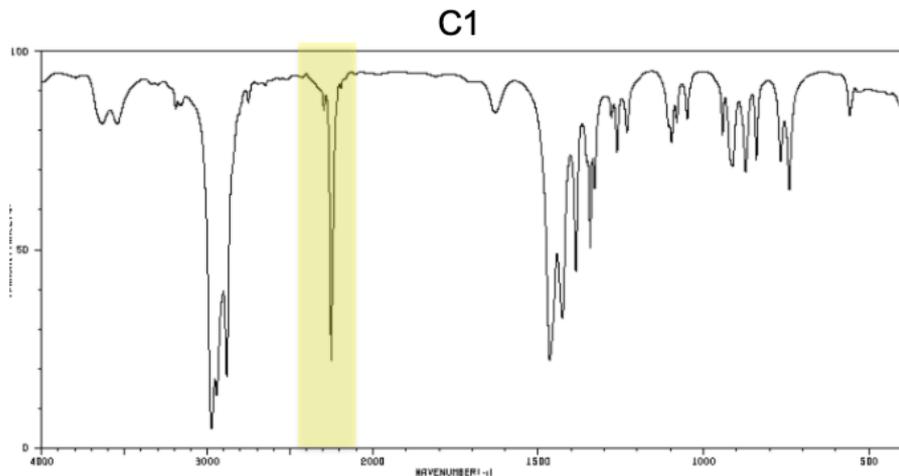
B3



B4



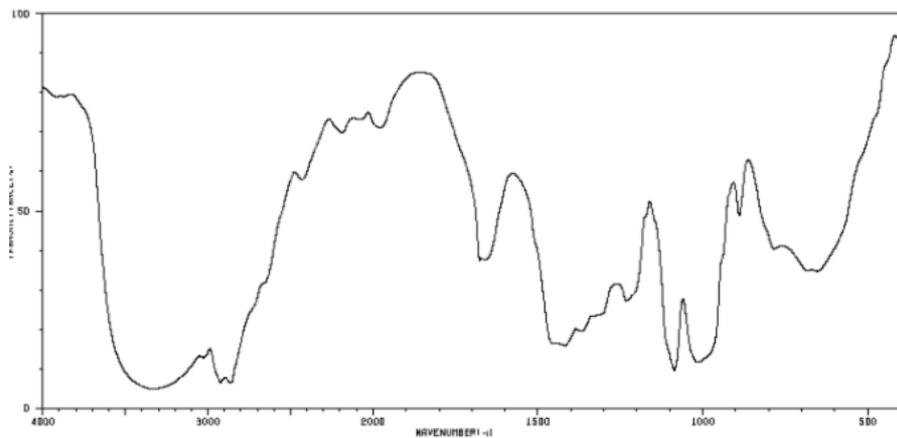
Which of these compounds contain a C≡N bond?



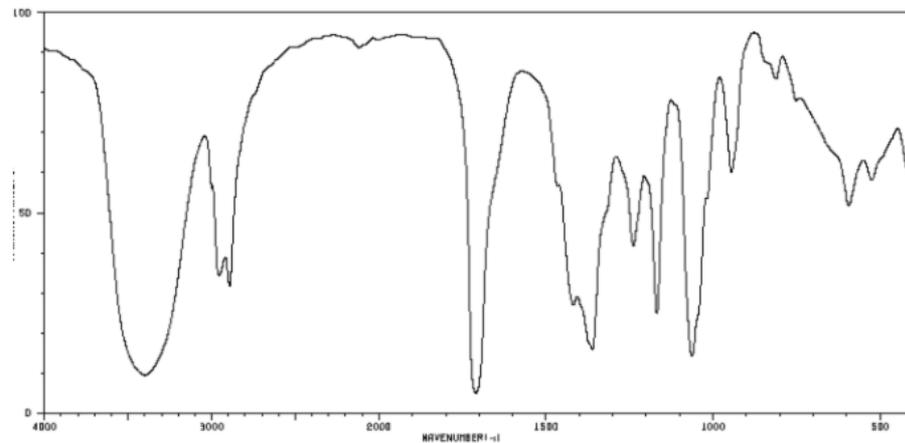
Acid O-H 2500-3000 cm^{-1}

Which of these compounds contain an O-H (acid) bond?

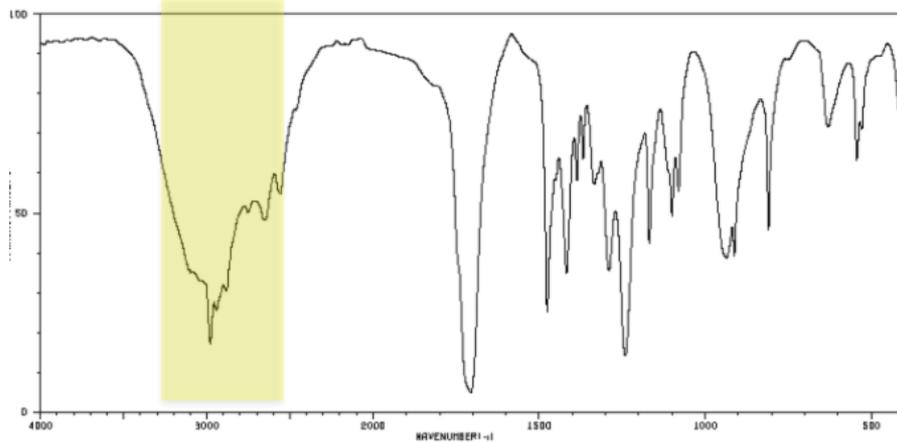
D1



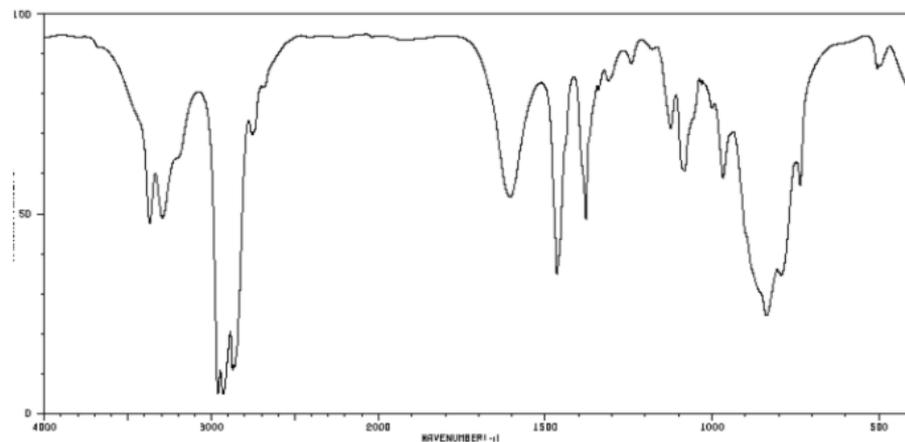
D2



D3



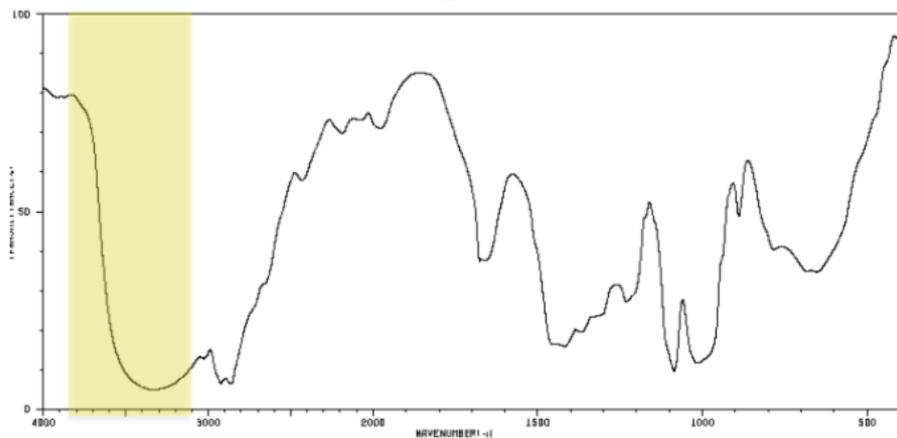
D4



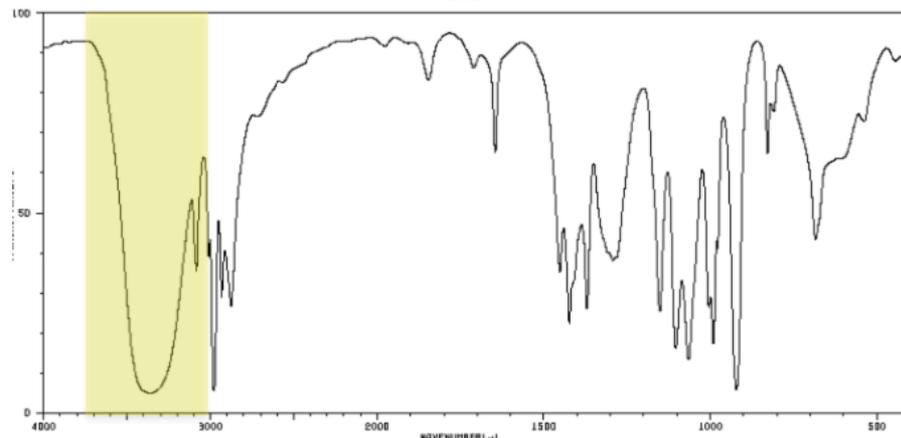
Alcohol O-H 3230-3550 cm^{-1}

Which of these compounds contain an O-H (alcohol) bond?

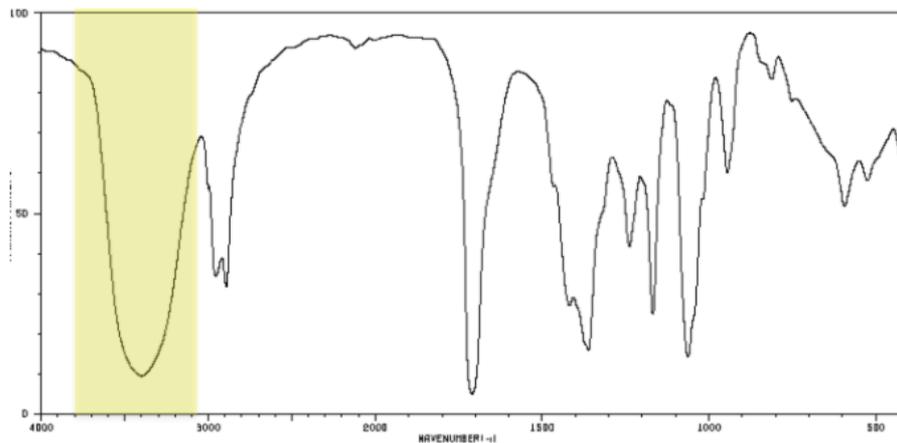
E1



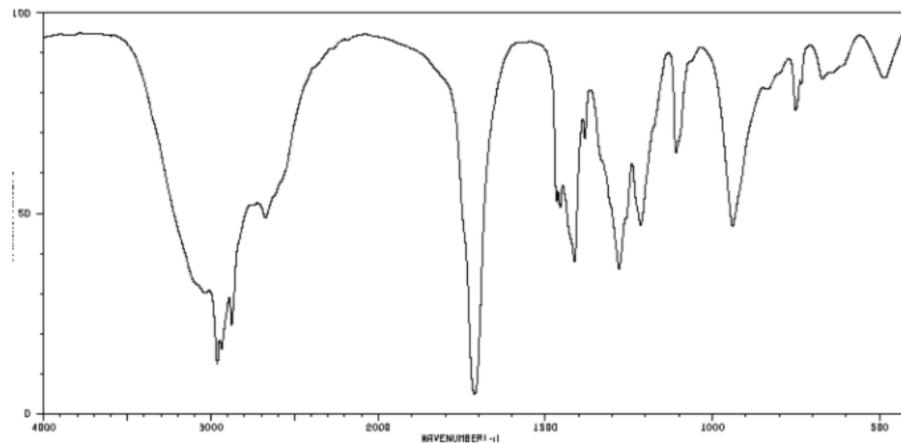
E2



E3



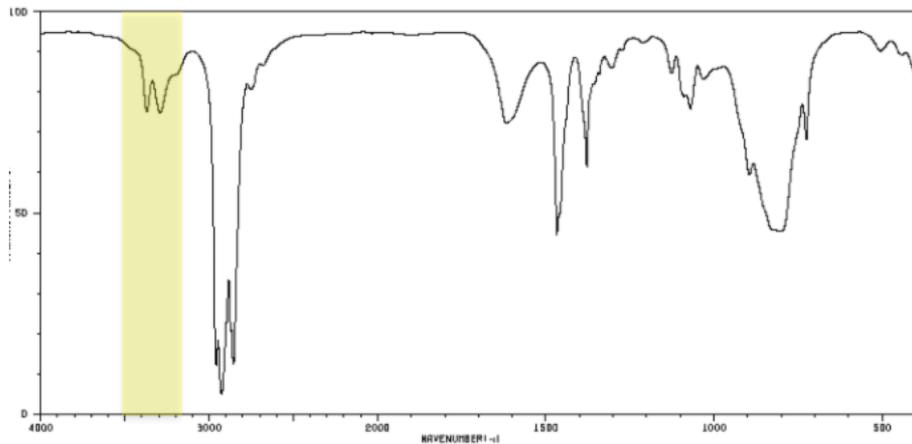
E4



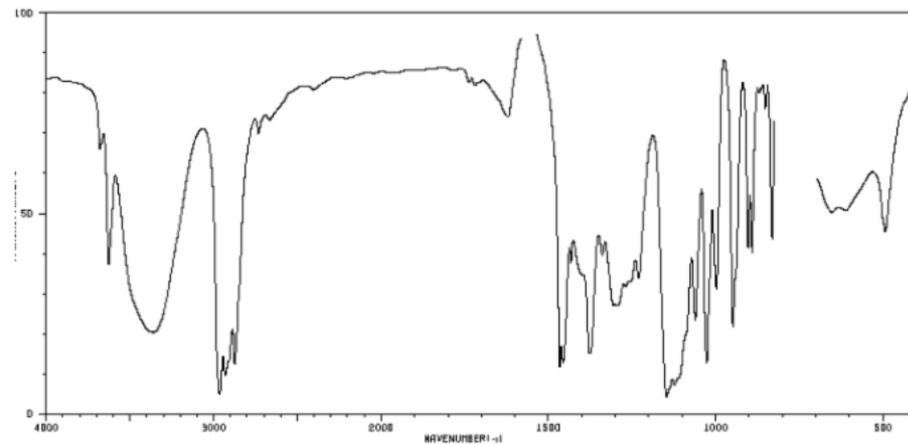
N-H 3300-3500 cm⁻¹

Which of these compounds contain an N-H (amine) bond?

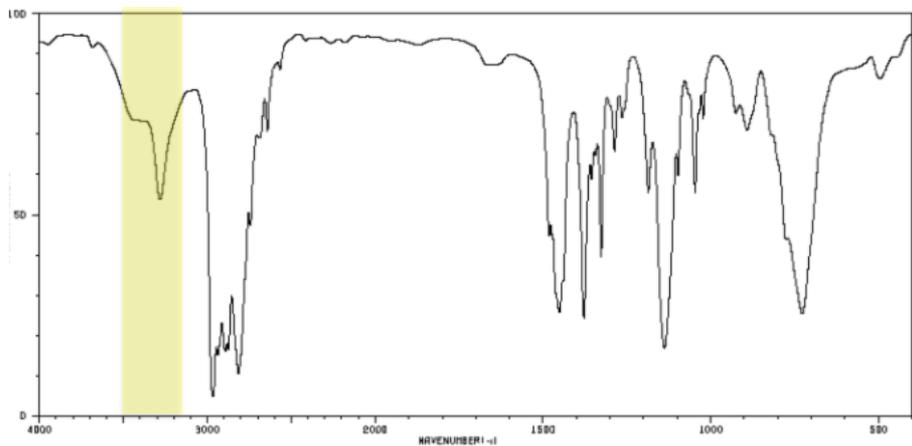
F1



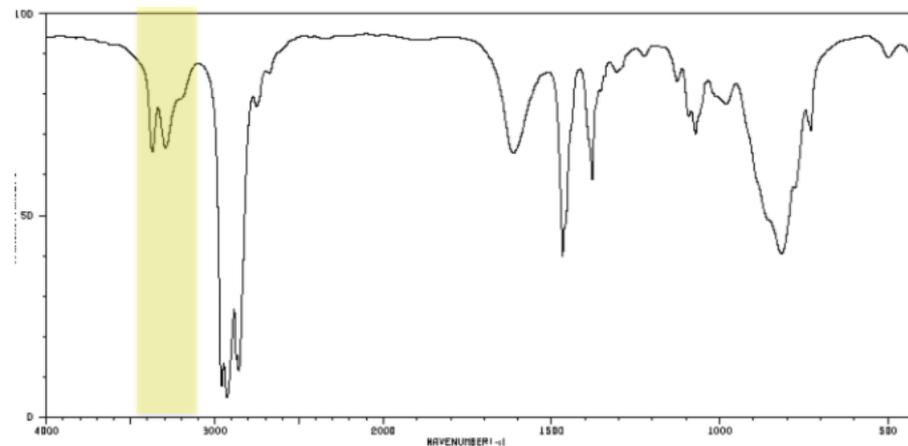
F2



F3

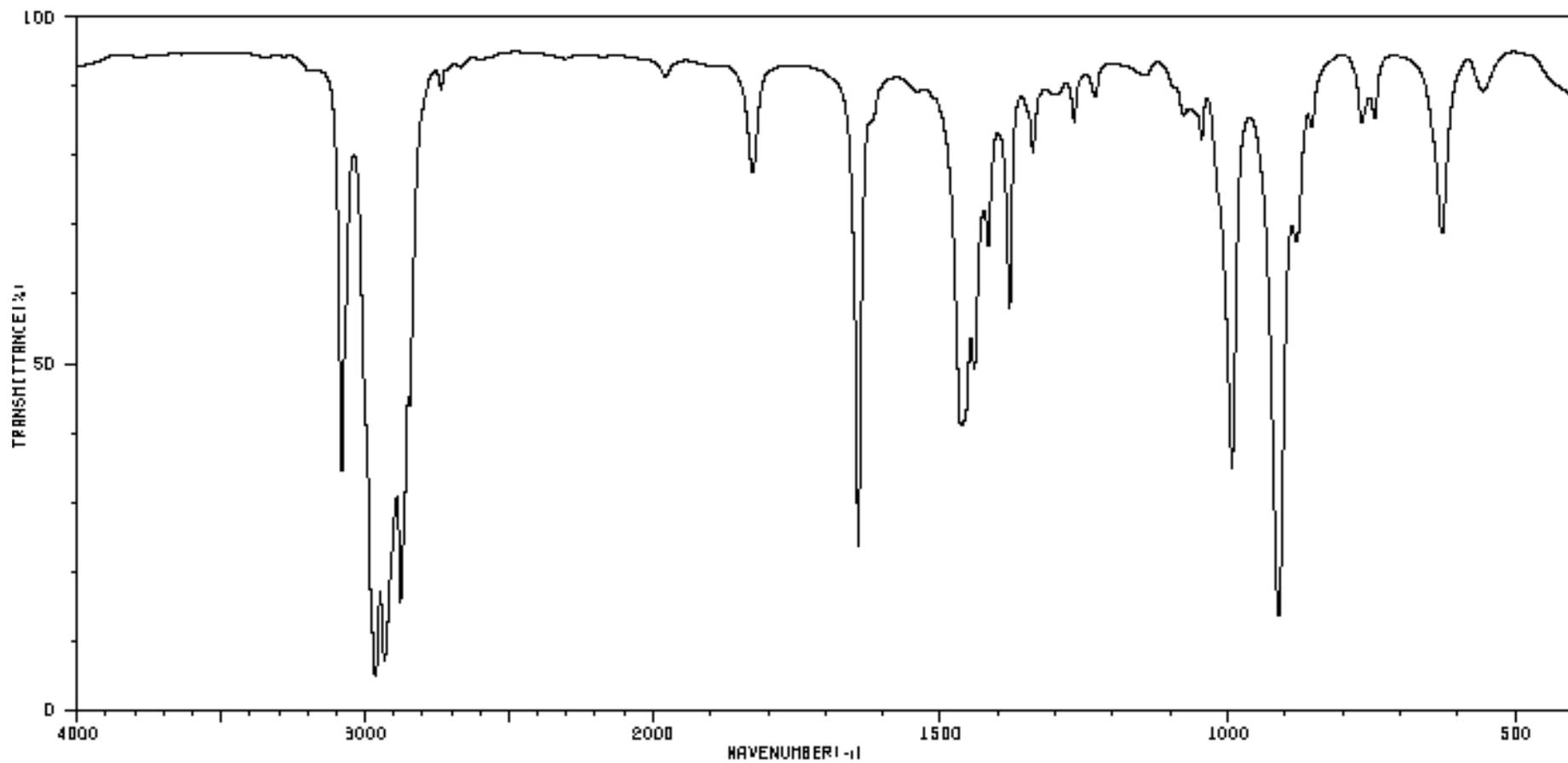


F4

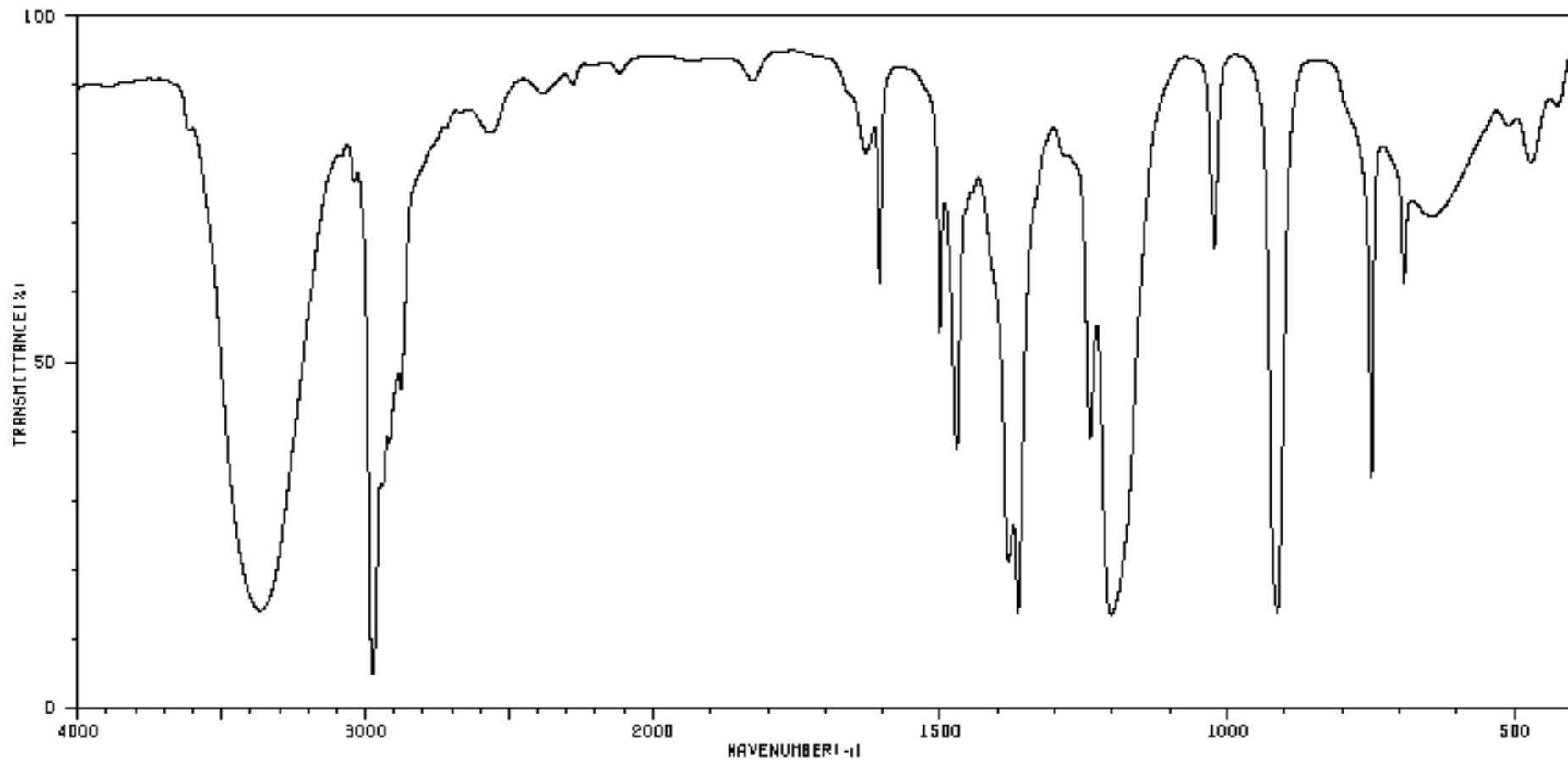


IR Problems E/1

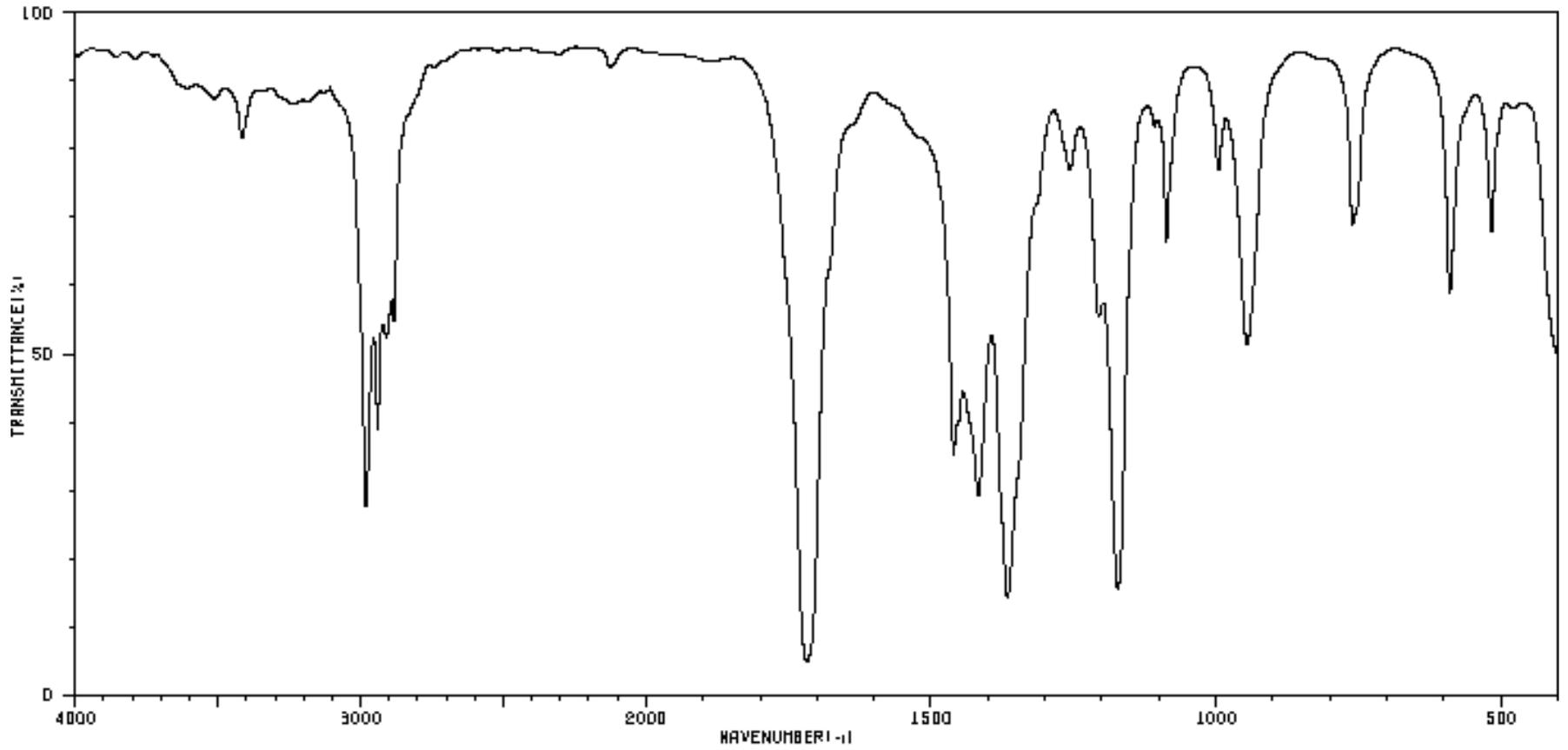
P



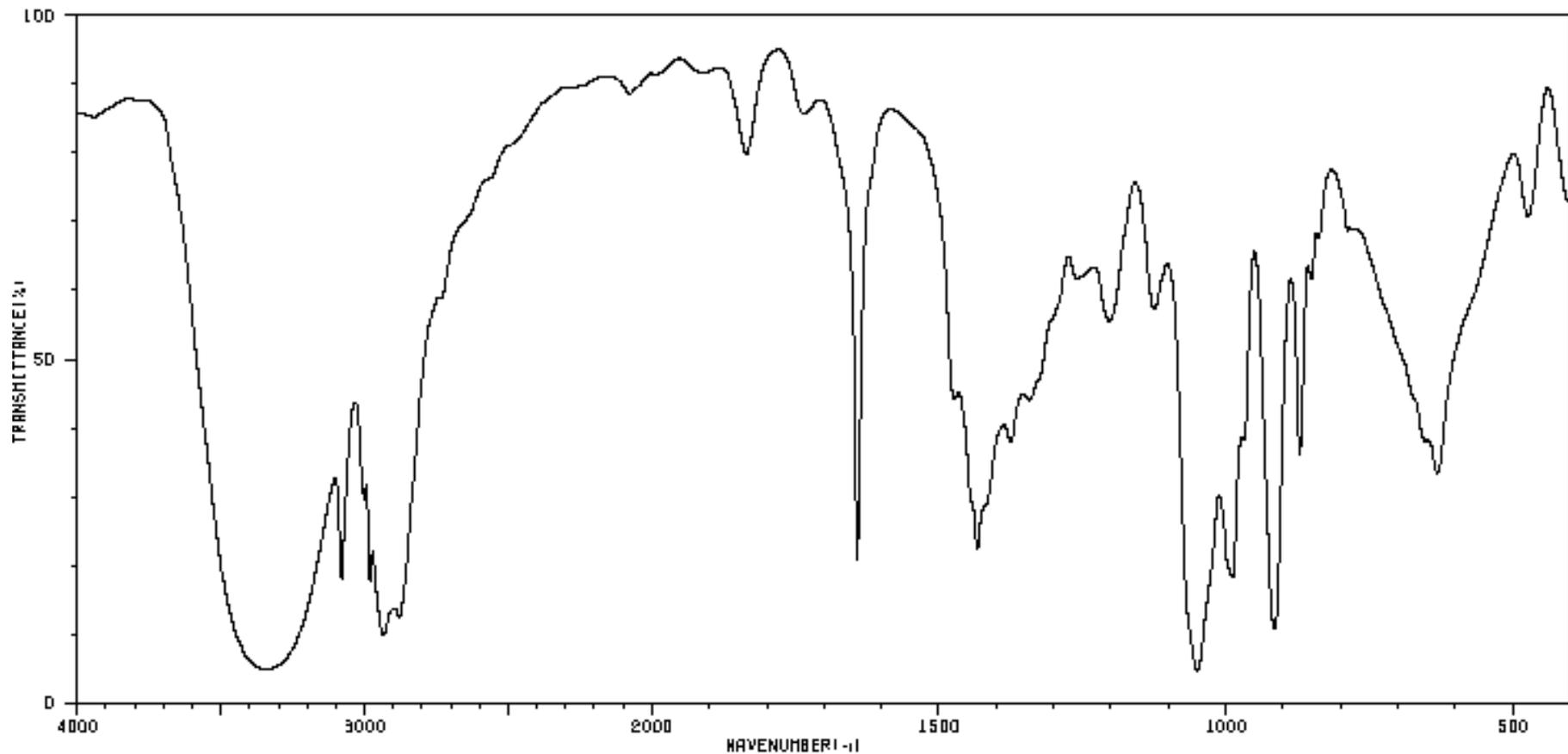
Q



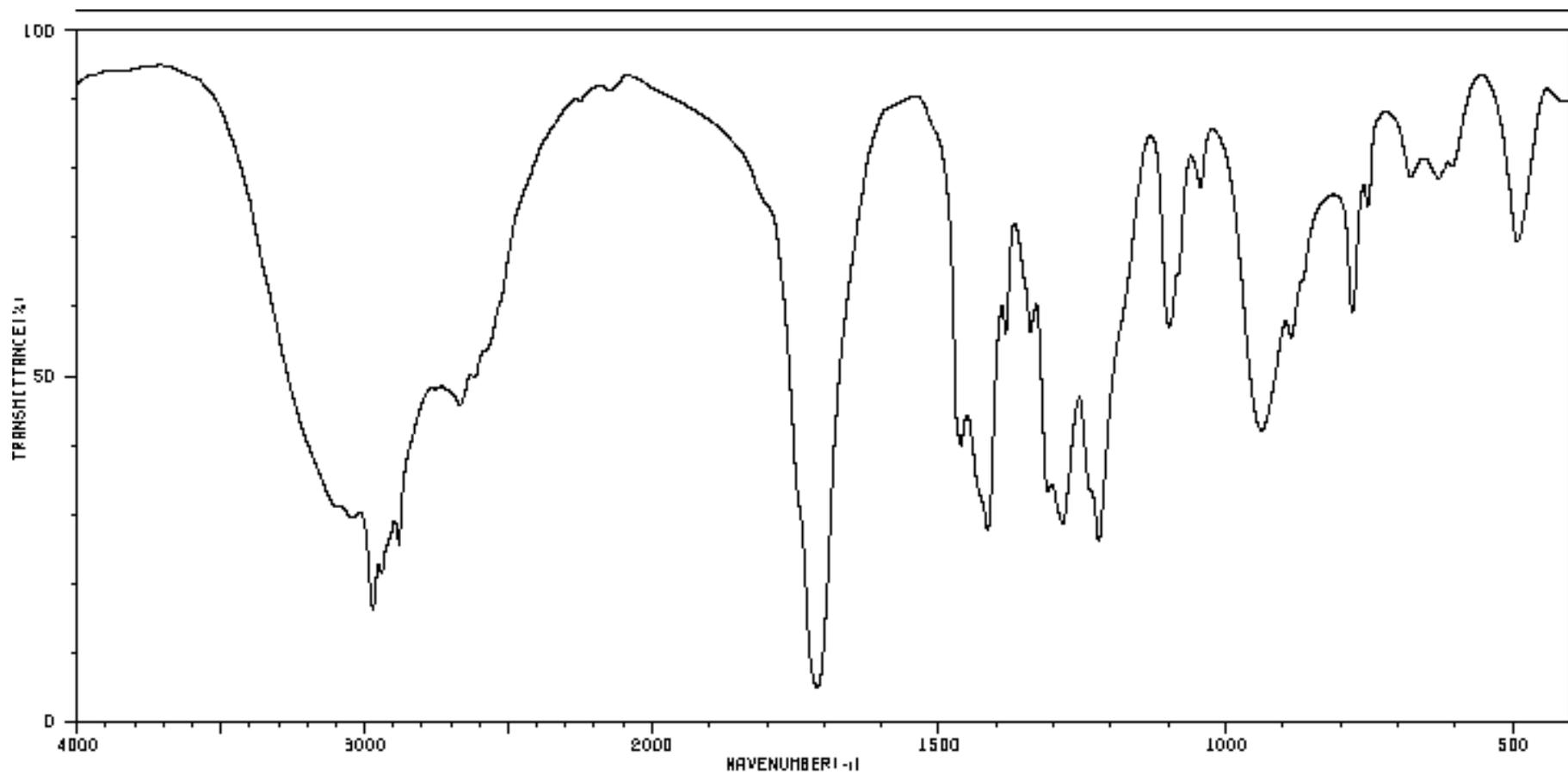
R



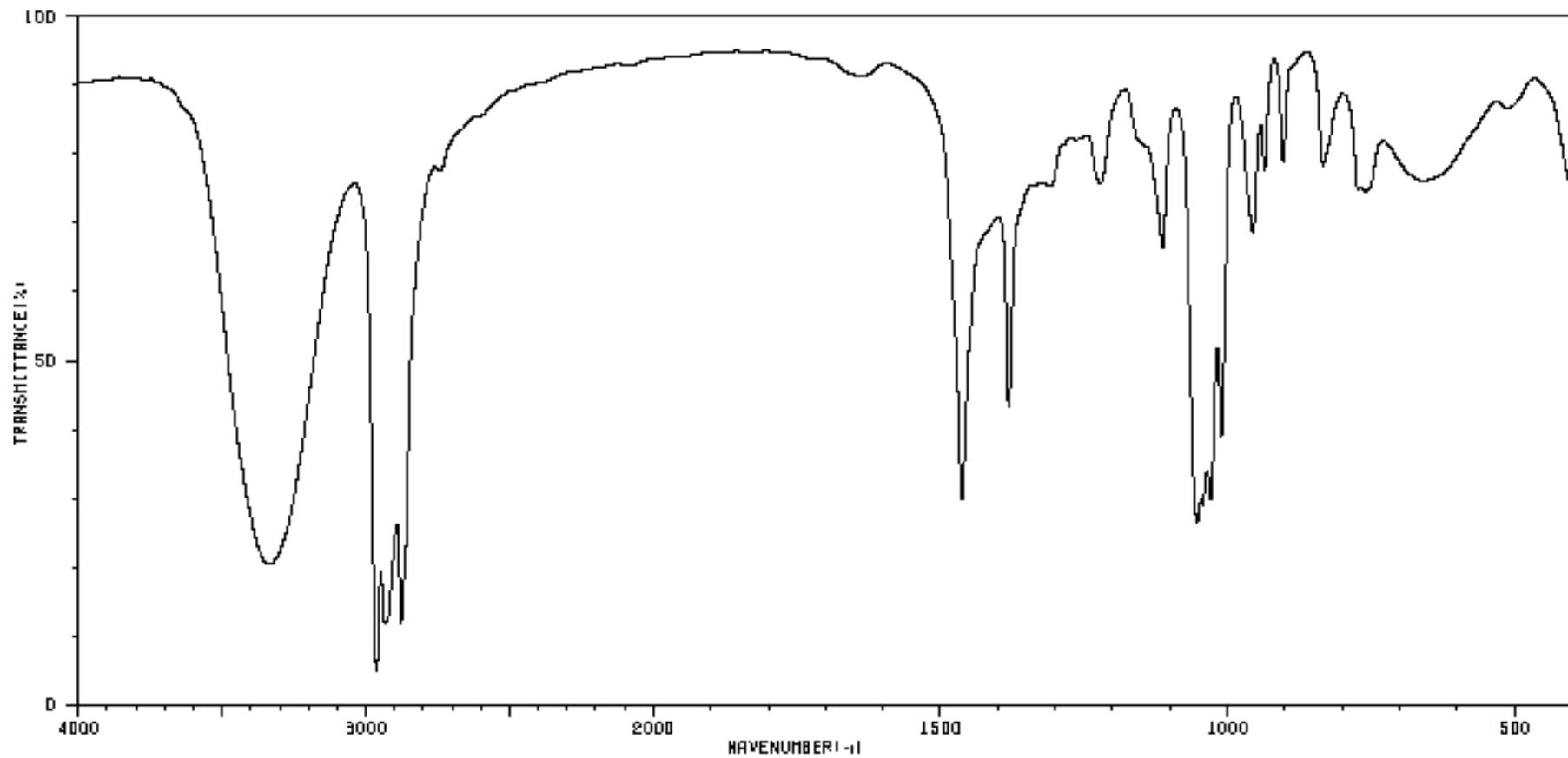
S



T

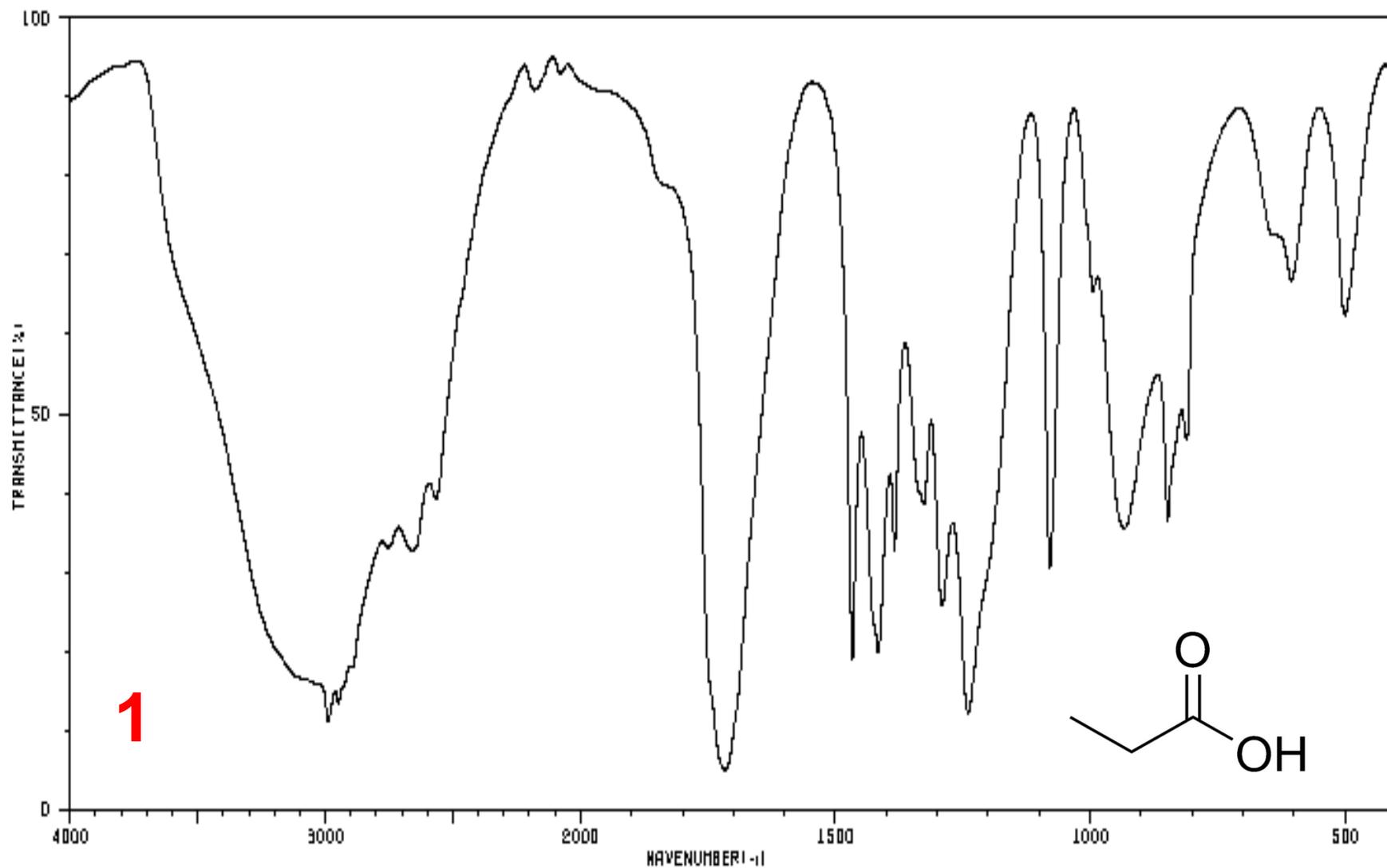


U



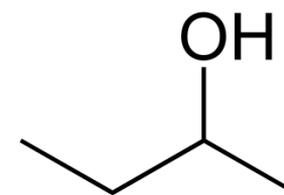
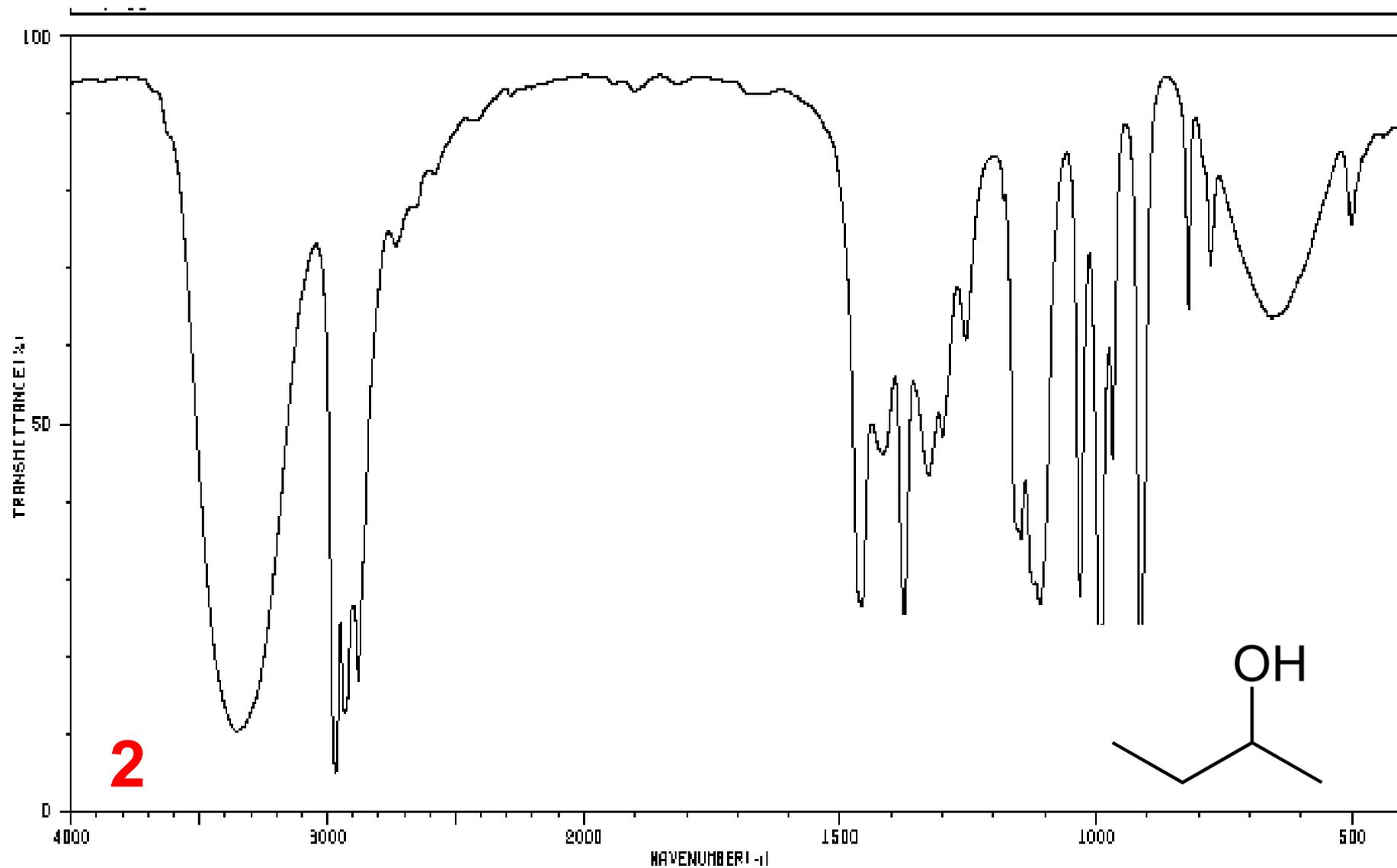
IR Problems D/2

propanoic acid, butanone, 2-methylbut-2-ene, 1-hydroxypropanone, butan-2-ol



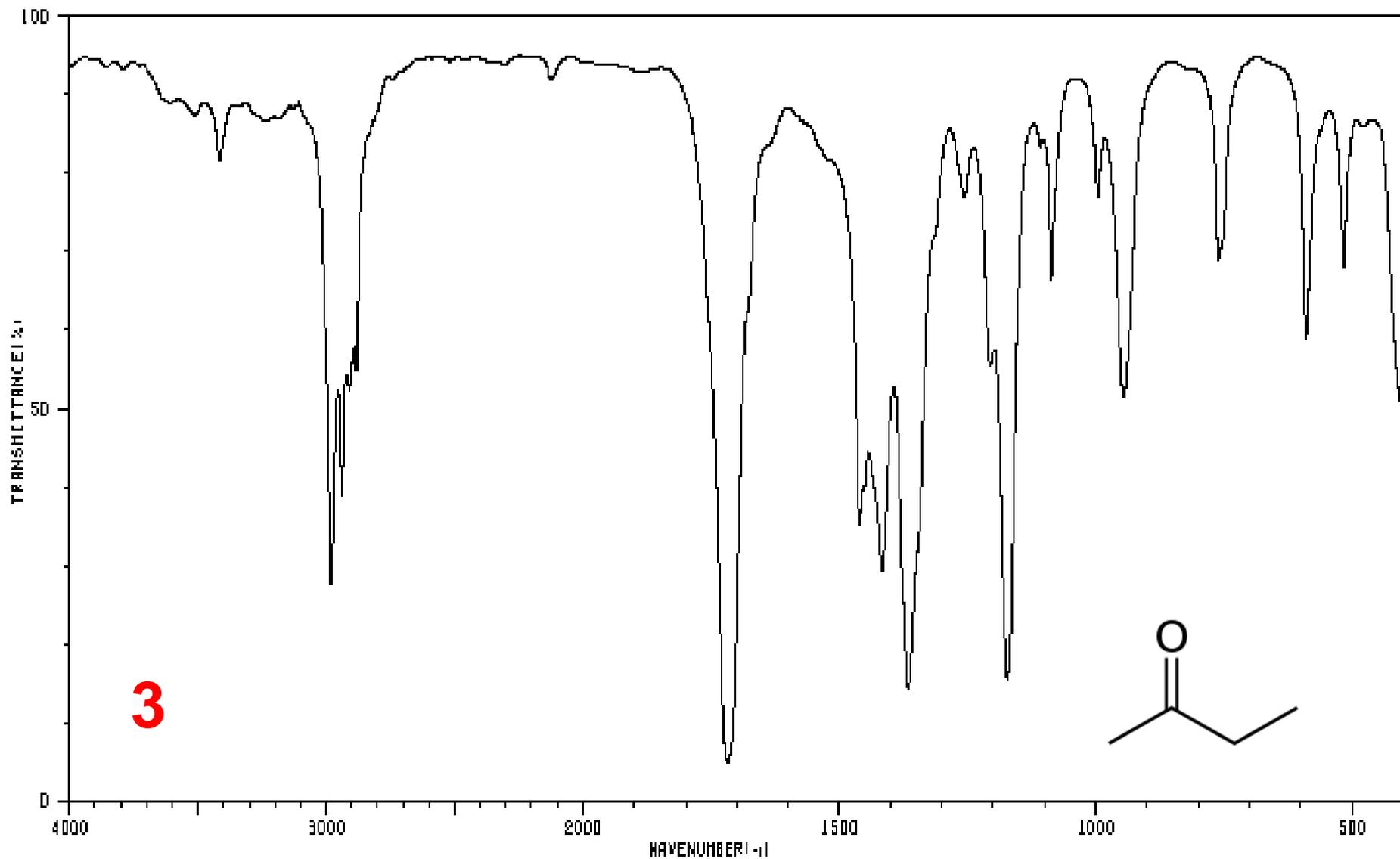
propanoic acid

propanoic acid, butanone, 2-methylbut-2-ene, 1-hydroxypropanone, butan-2-ol



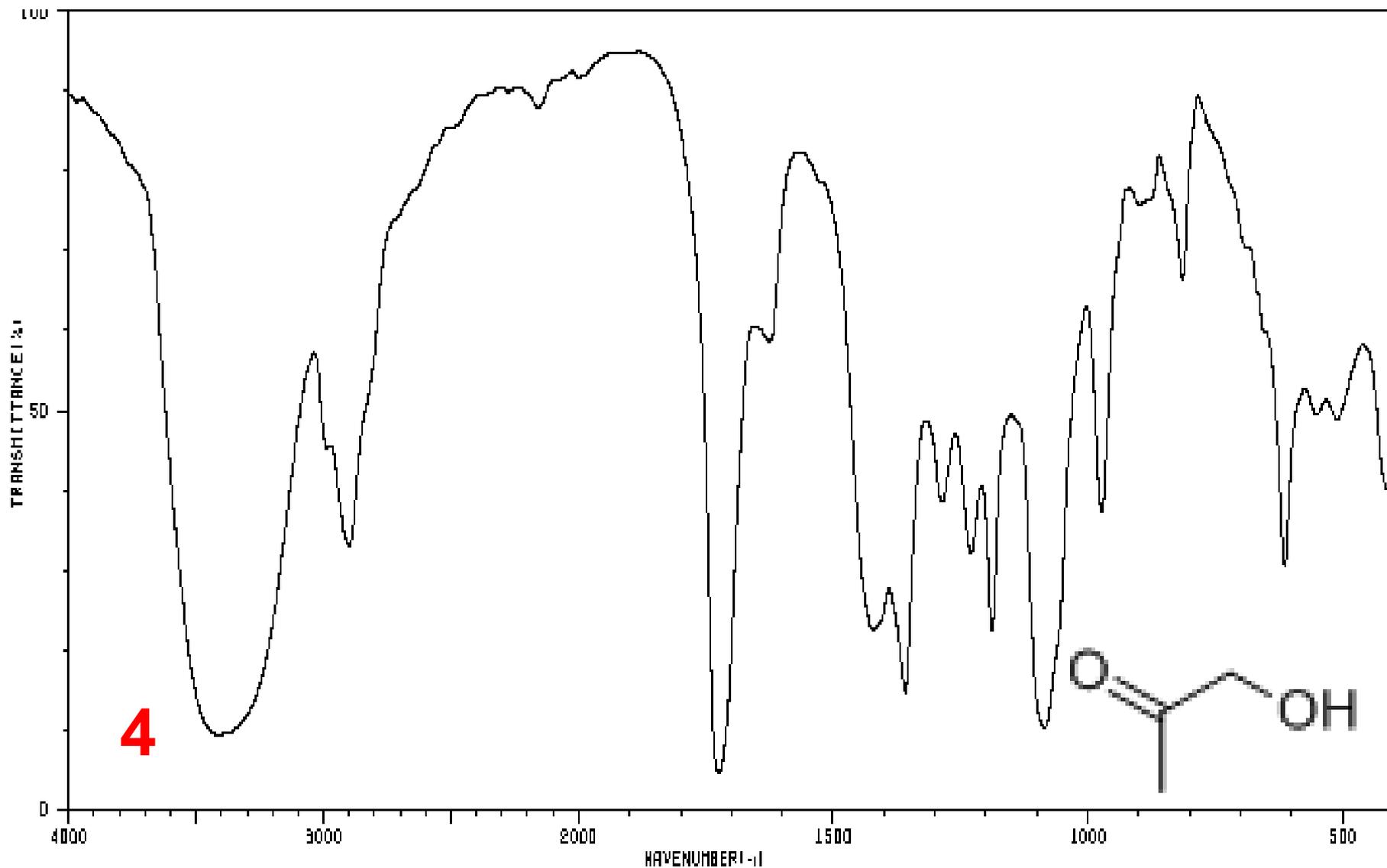
butan-2-ol

propanoic acid, butanone, 2-methylbut-2-ene, 1-hydroxypropanone, butan-2-ol



butanone

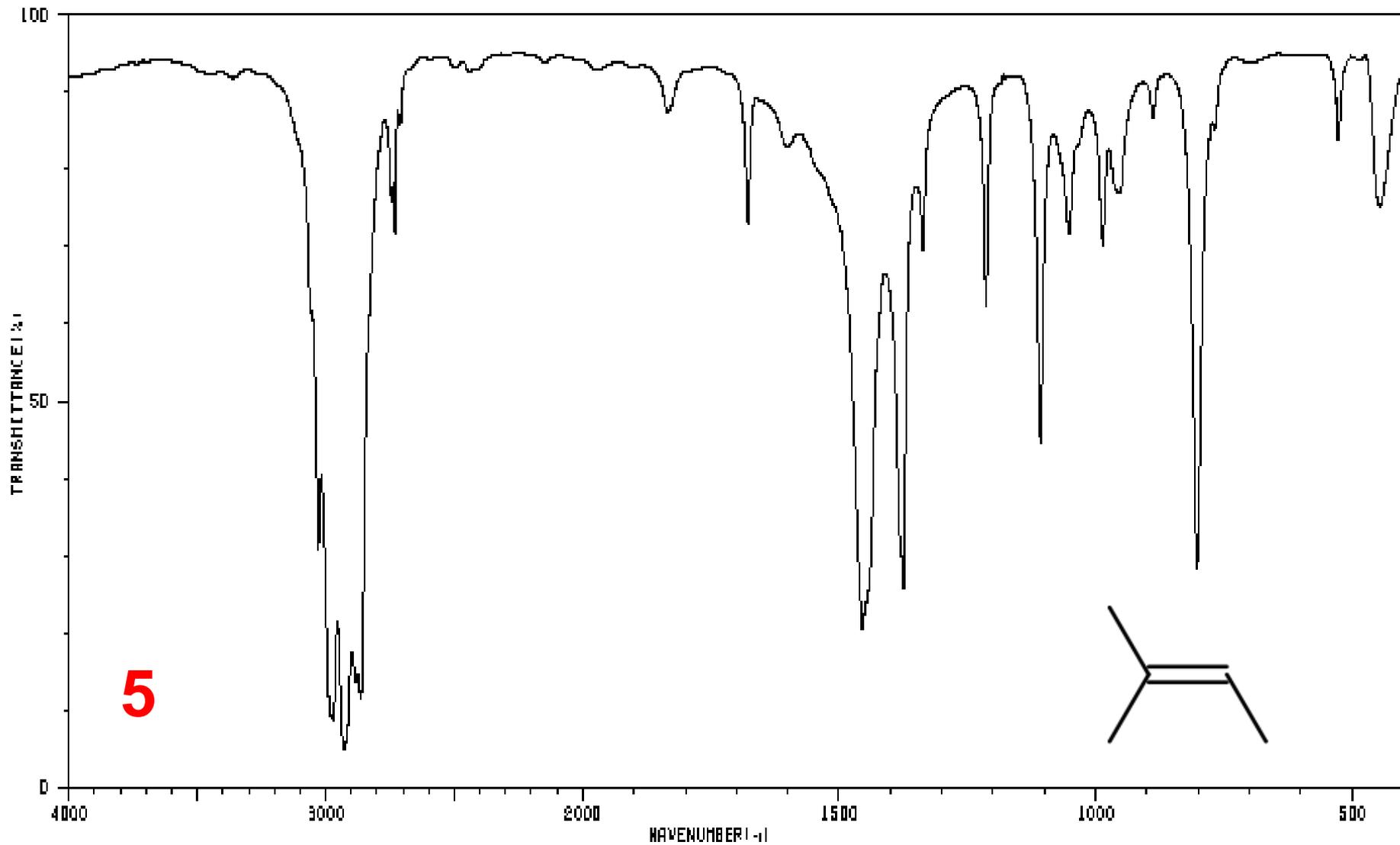
propanoic acid, butanone, 2-methylbut-2-ene, 1-hydroxypropanone, butan-2-ol



4

1-hydroxypropanone

propanoic acid, butanone, 2-methylbut-2-ene, 1-hydroxypropanone, butan-2-ol



2-methylbut-2-ene

IR Problems C/3

hex-2-ene

butanal

pentane

butanoic acid

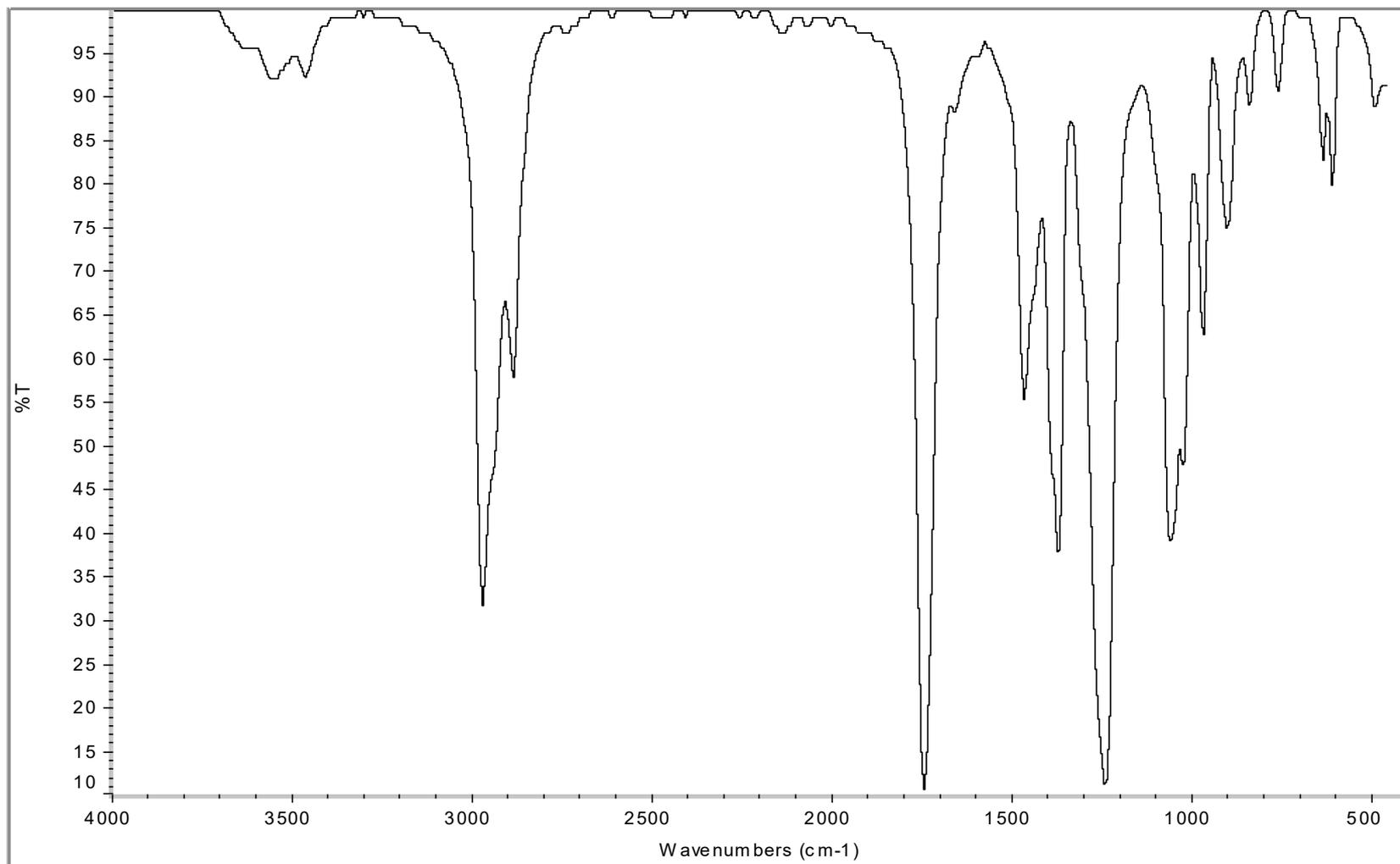
methylpropan-1-ol

propyl ethanoate

2-methylpentan-3-one

butanenitrile

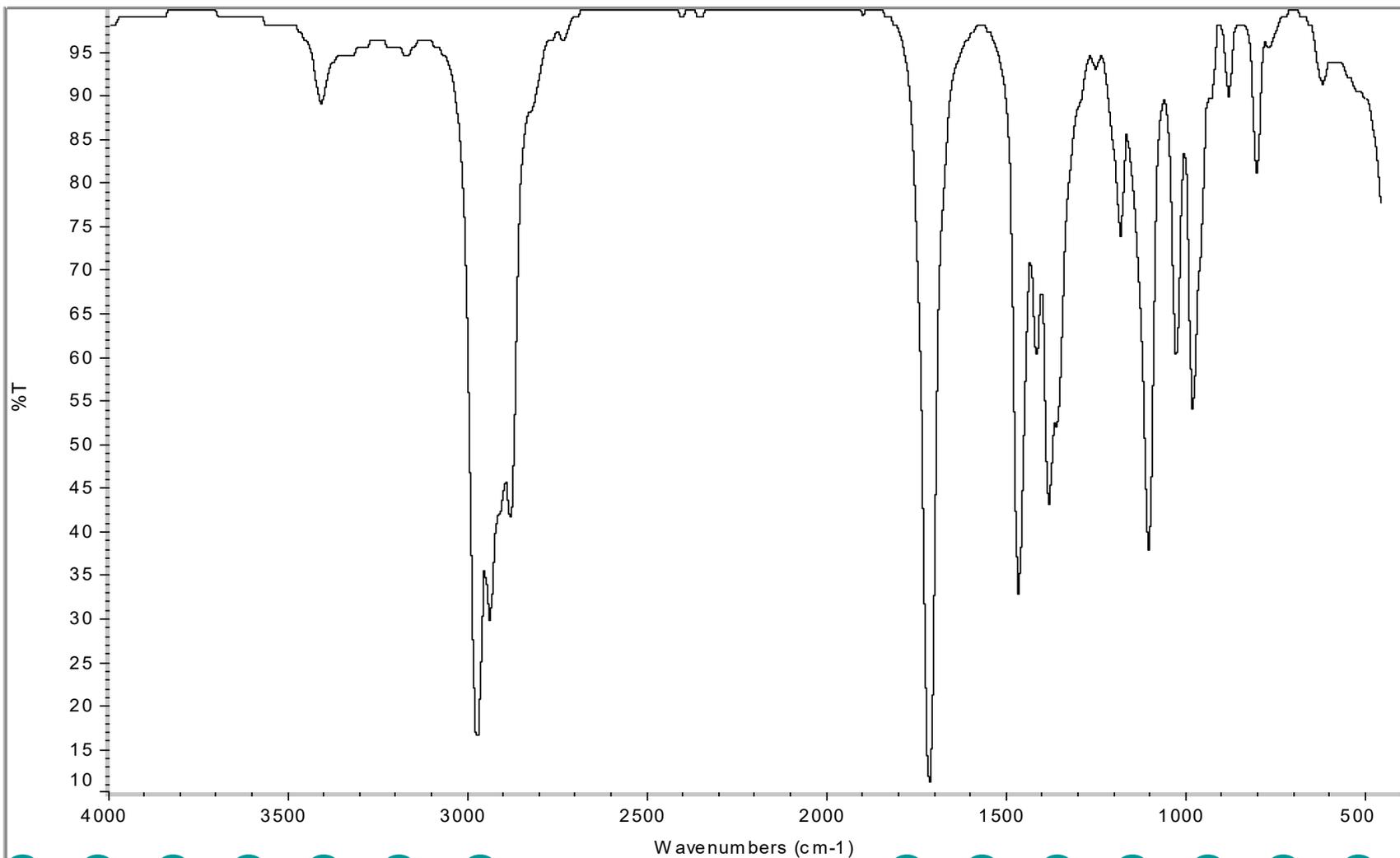
1



1 2 3 4 5 6 7 8

1 2 3 4 5 6 7 8

2



1

2

3

4

5

6

7

8

1

2

3

4

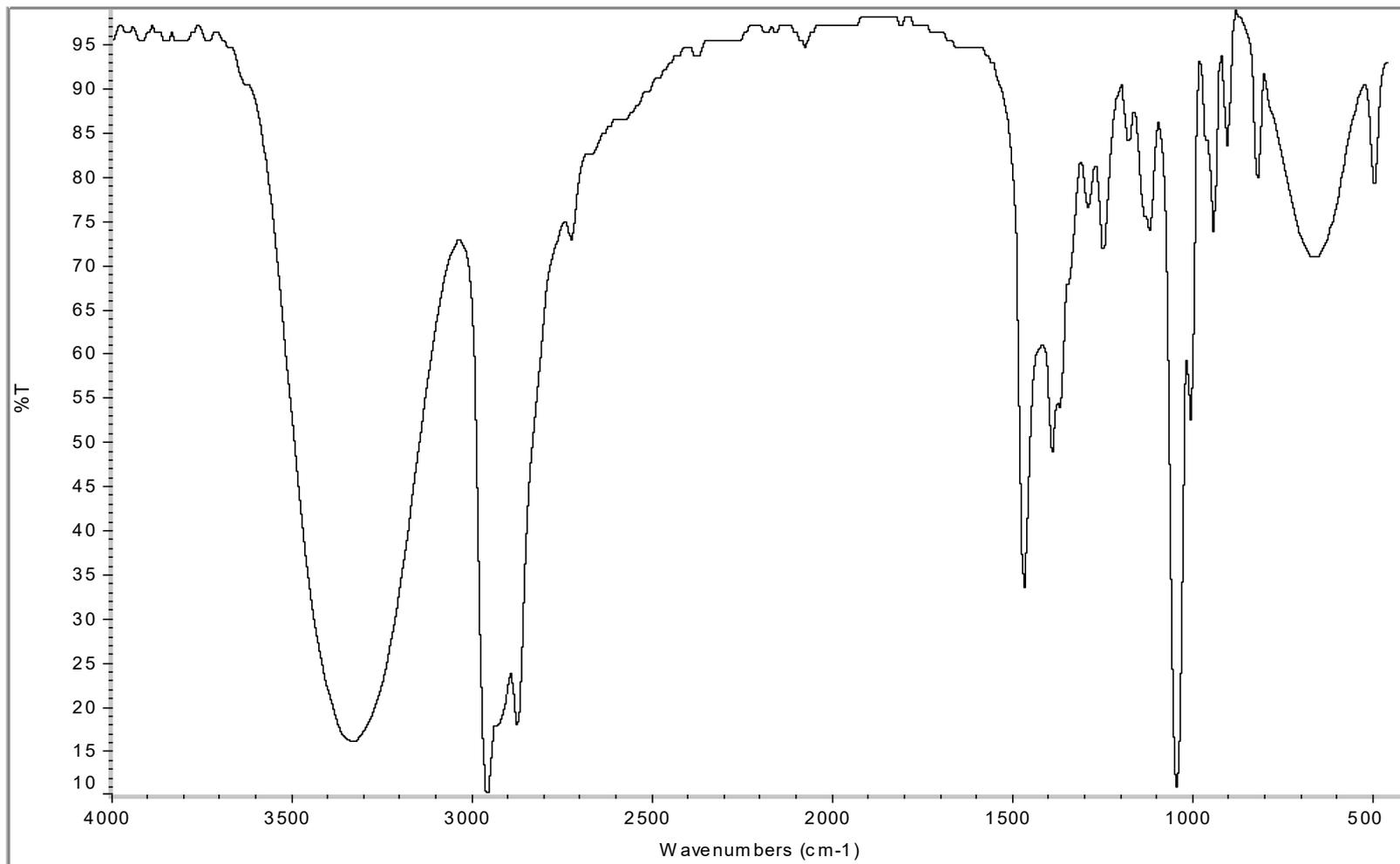
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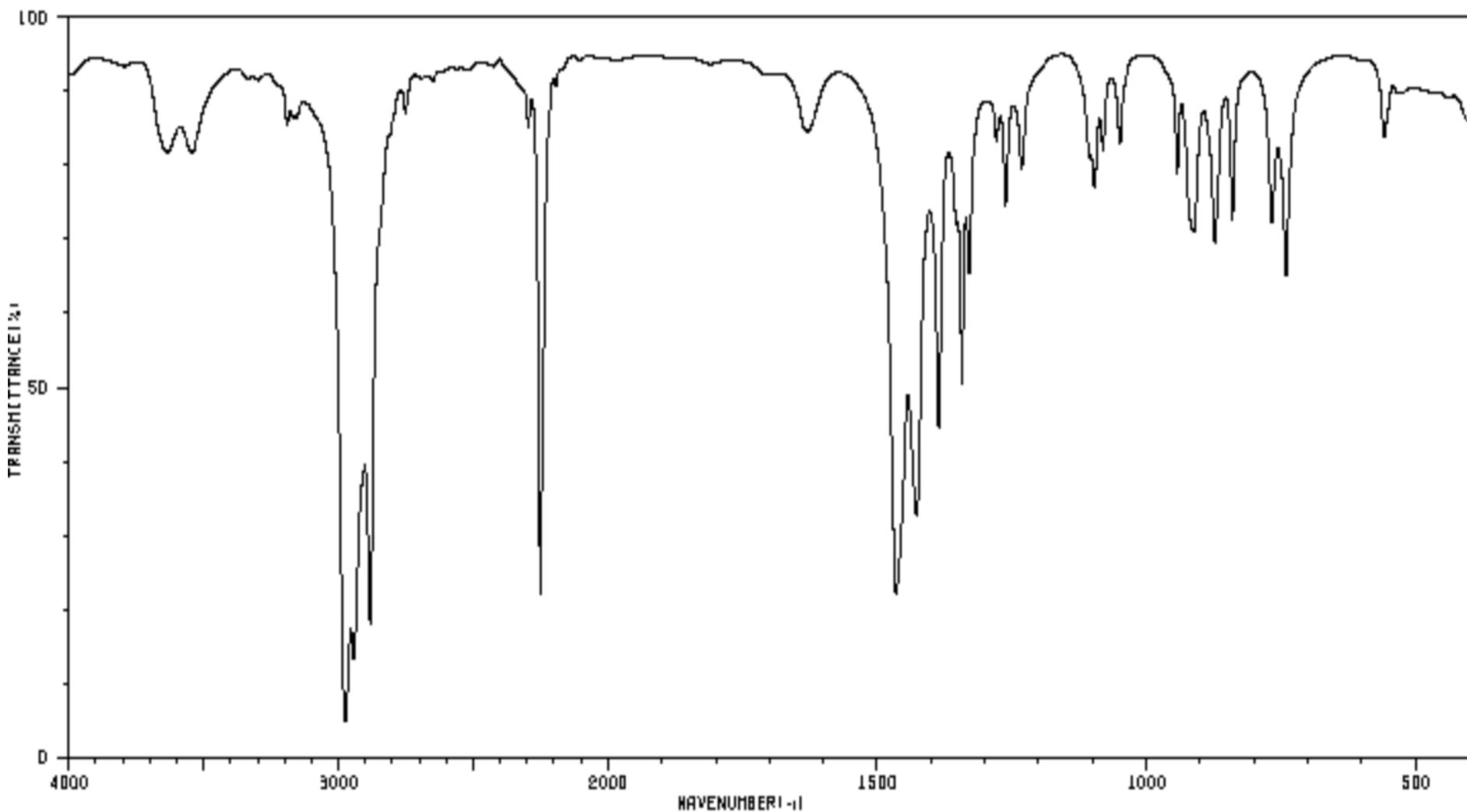
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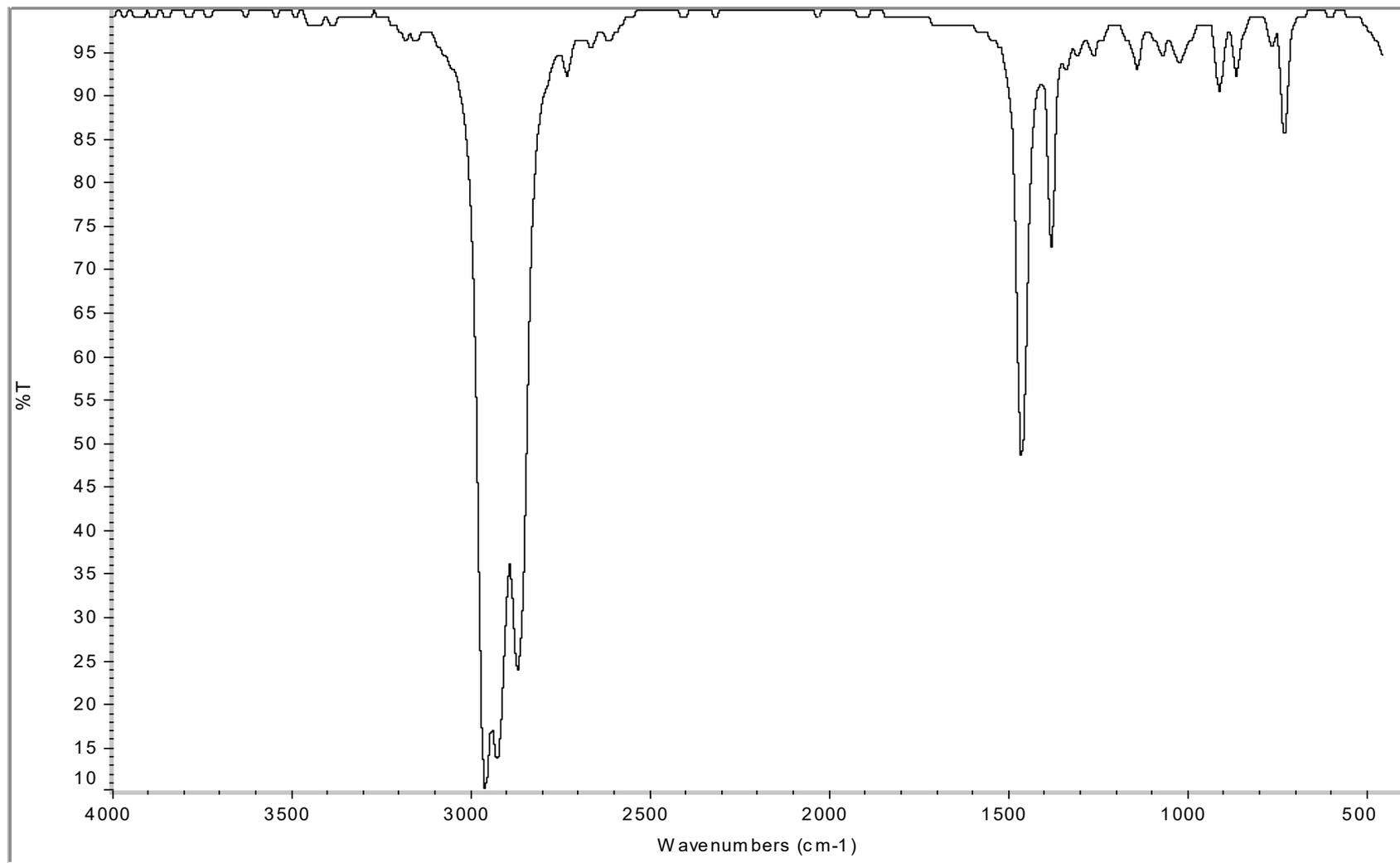
4



- 1
- 2
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- 5
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- 7
- 8

- 1
- 2
- 3
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- 5
- 6
- 7
- 8

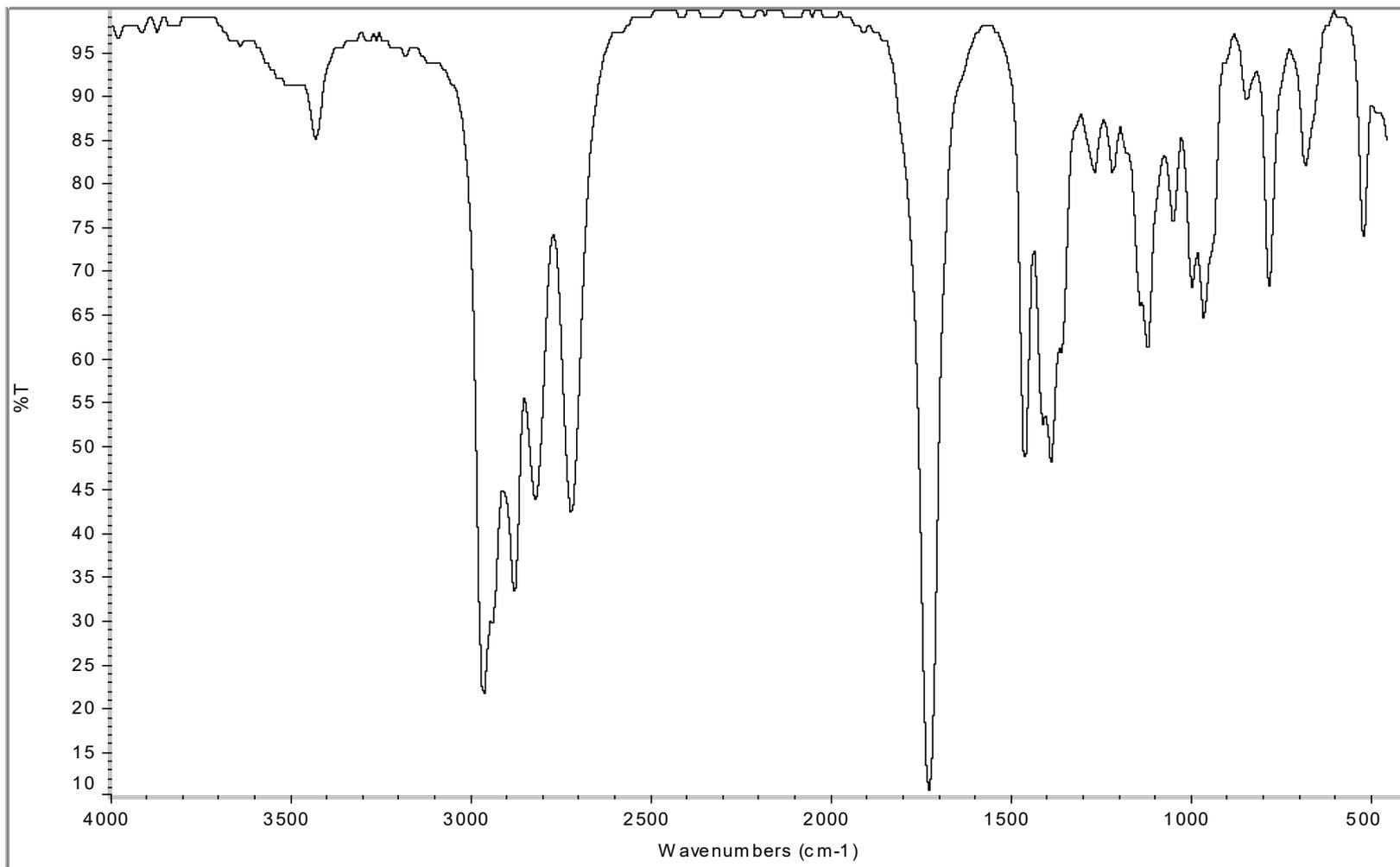
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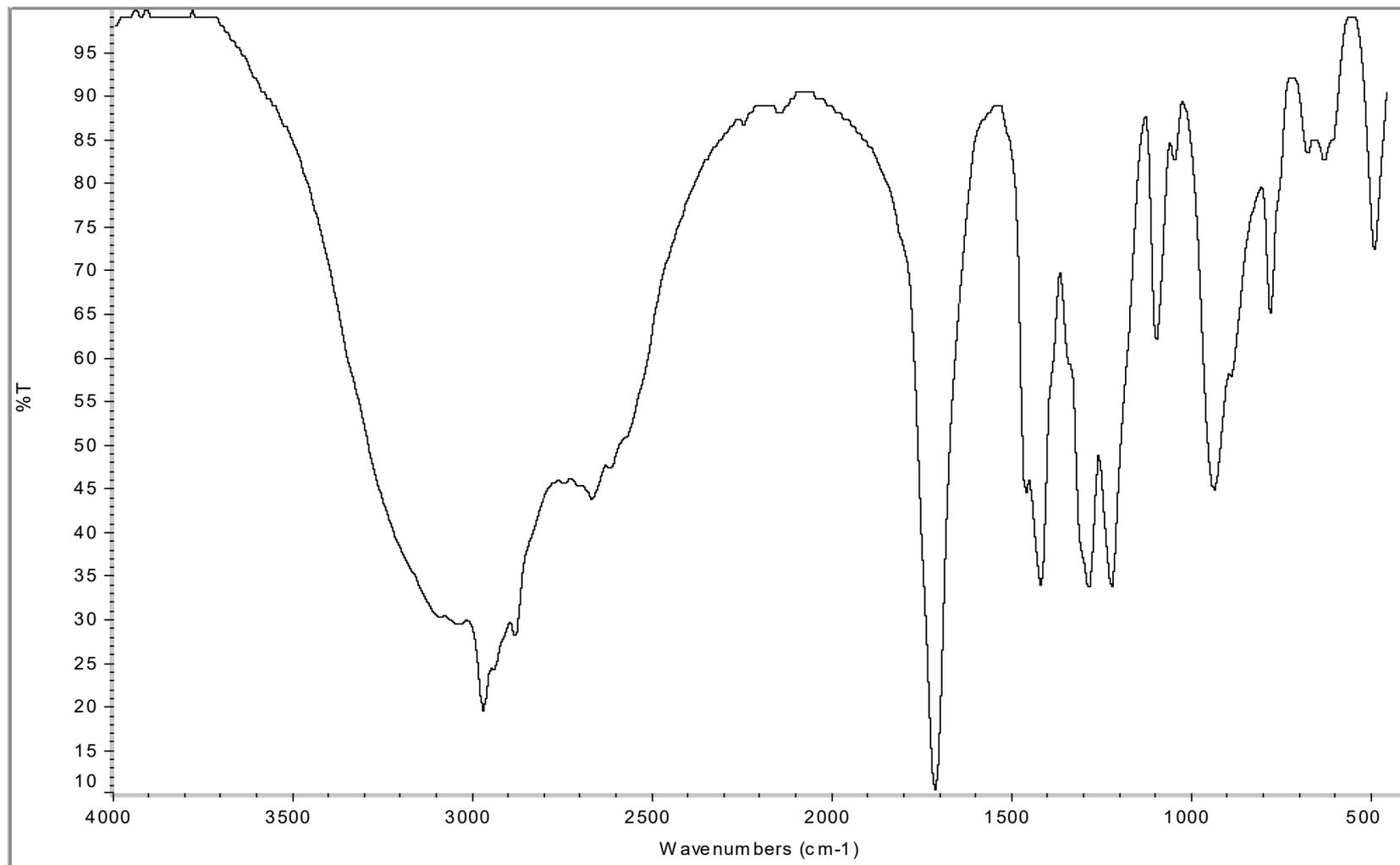
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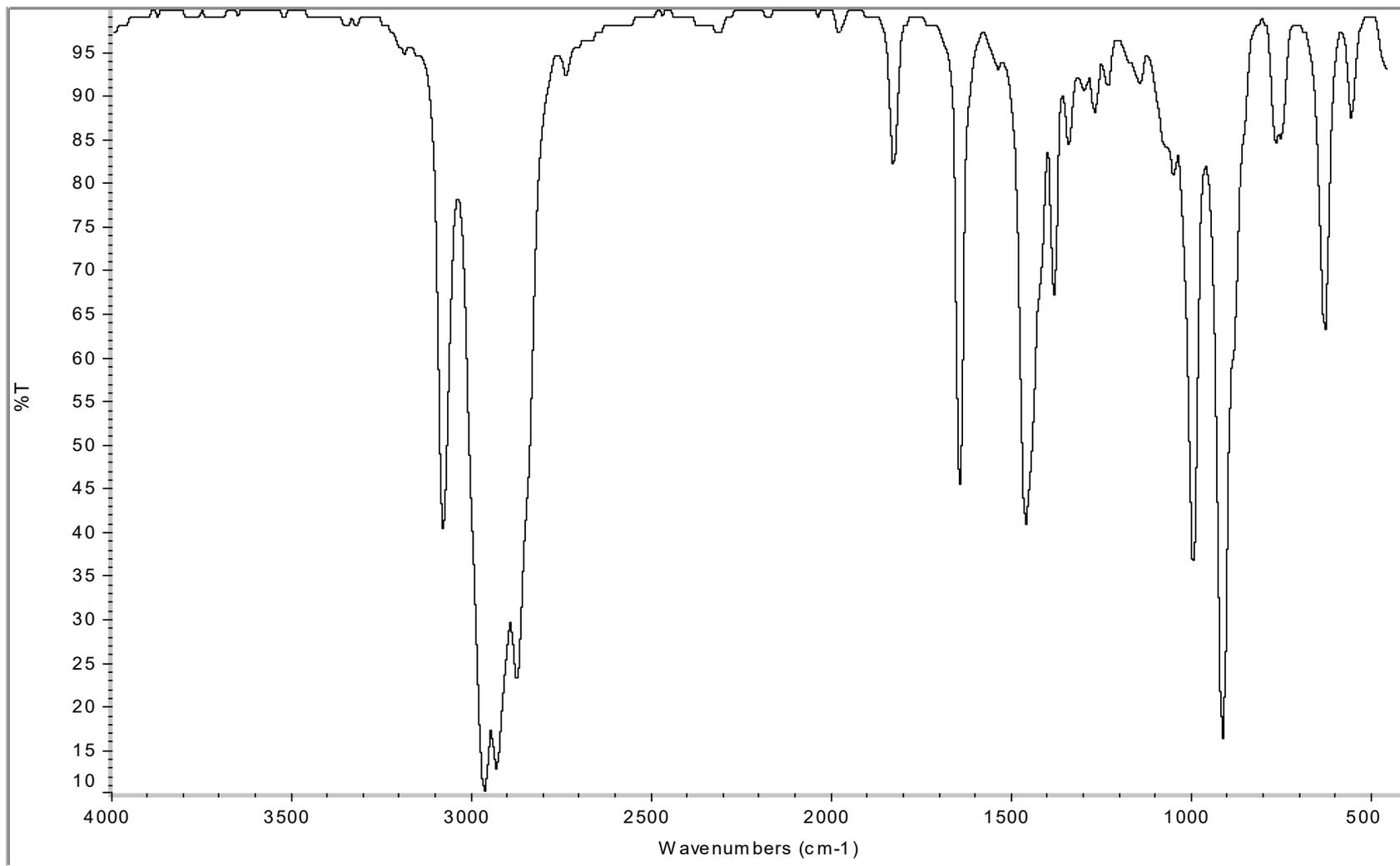
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1 2 3 4 5 6 7 8

8

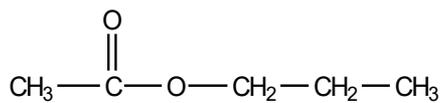


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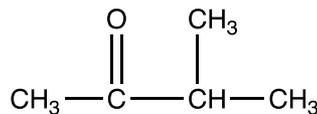
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propyl ethanoate



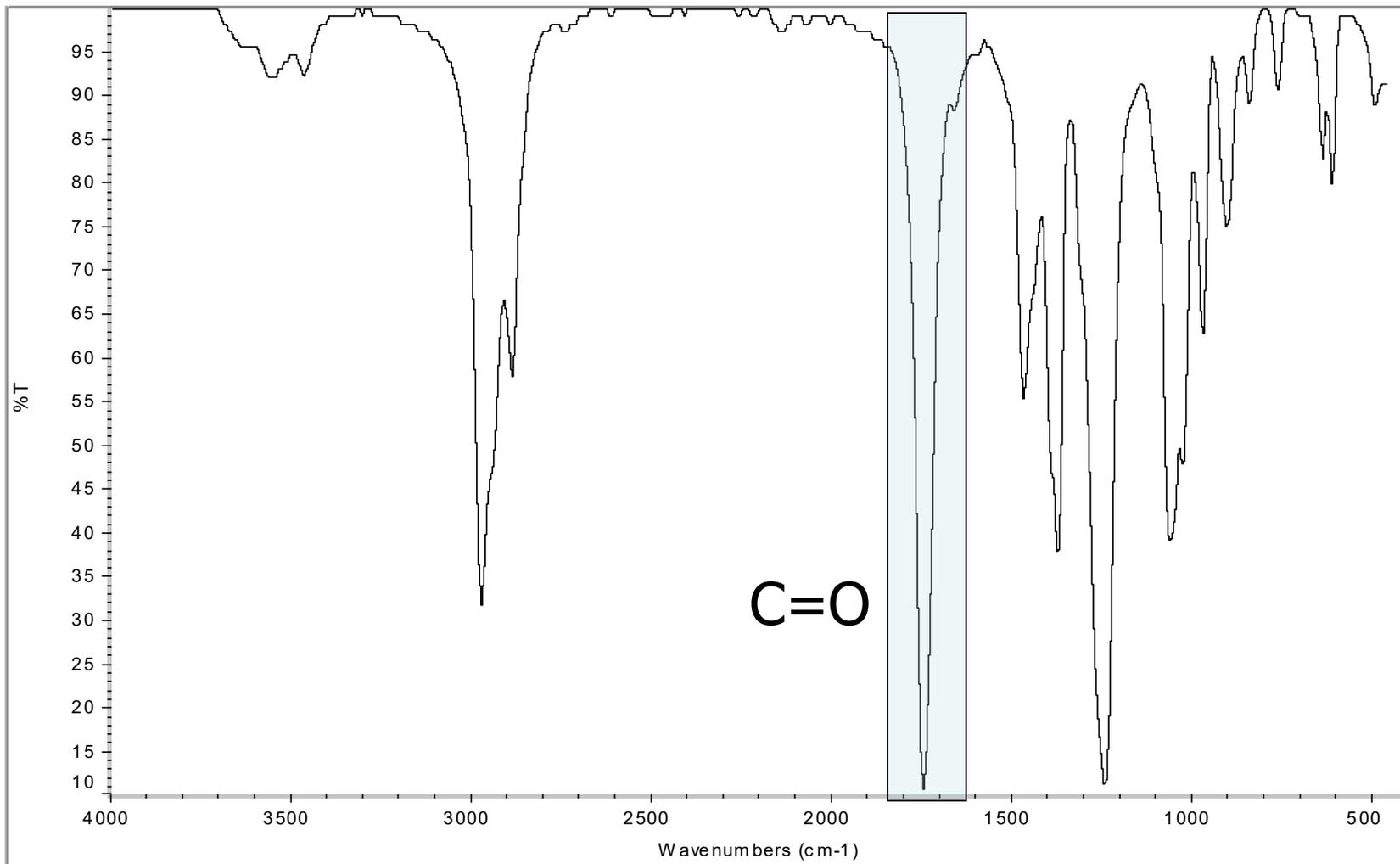
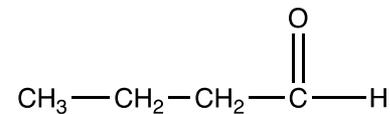
OR

2-methylpentan-3-one



OR

butanal

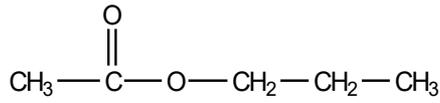


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1 2 3 4 5 6 7 8

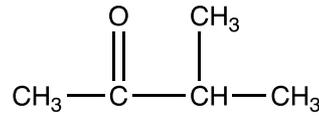
2

propyl ethanoate



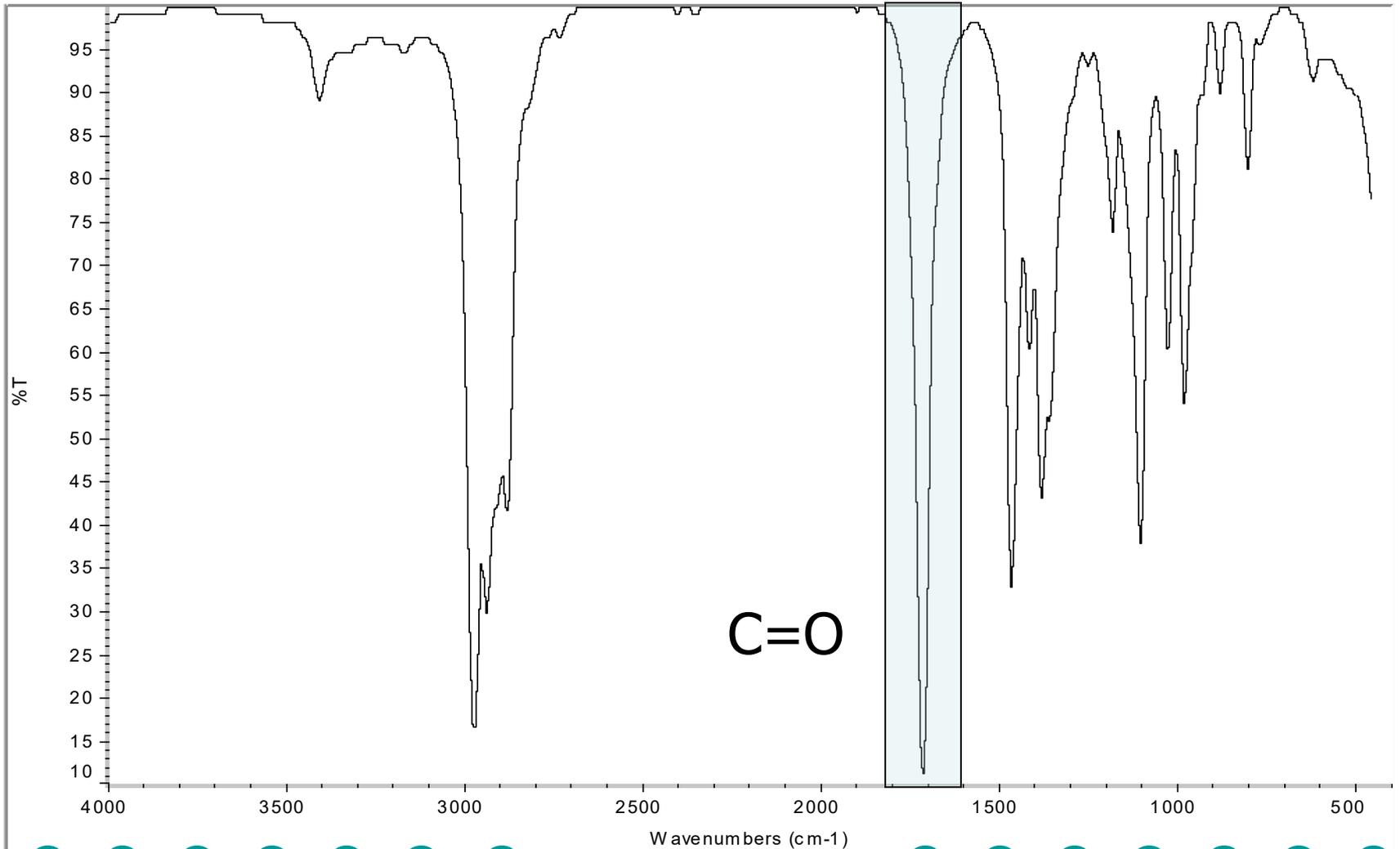
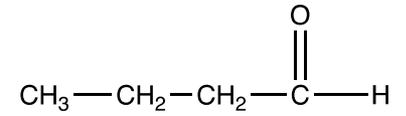
OR

2-methylpentan-3-one



OR

butanal

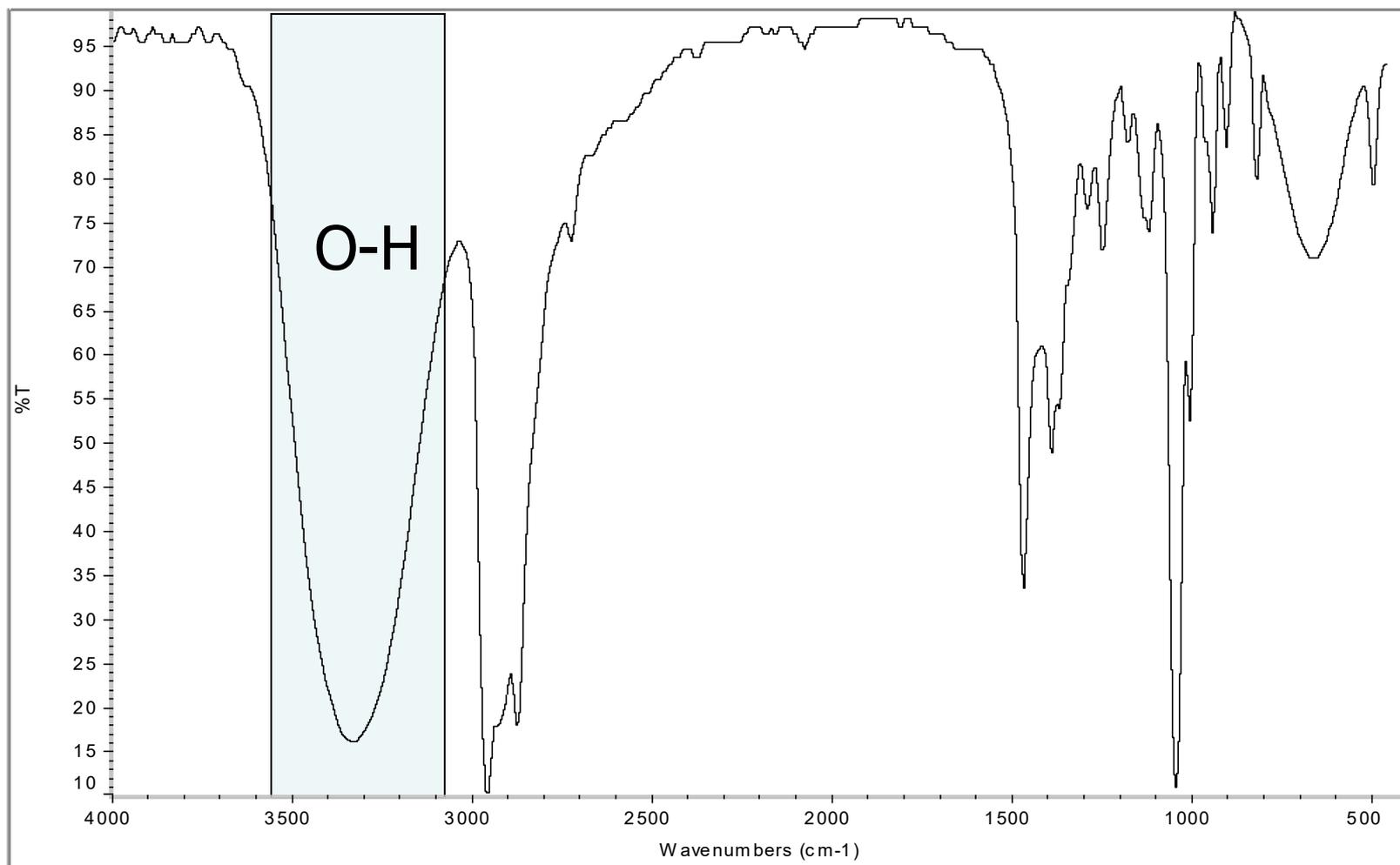
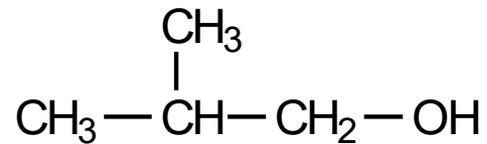


1 2 3 4 5 6 7 8

1 2 3 4 5 6 7 8

3

methylpropan-1-ol

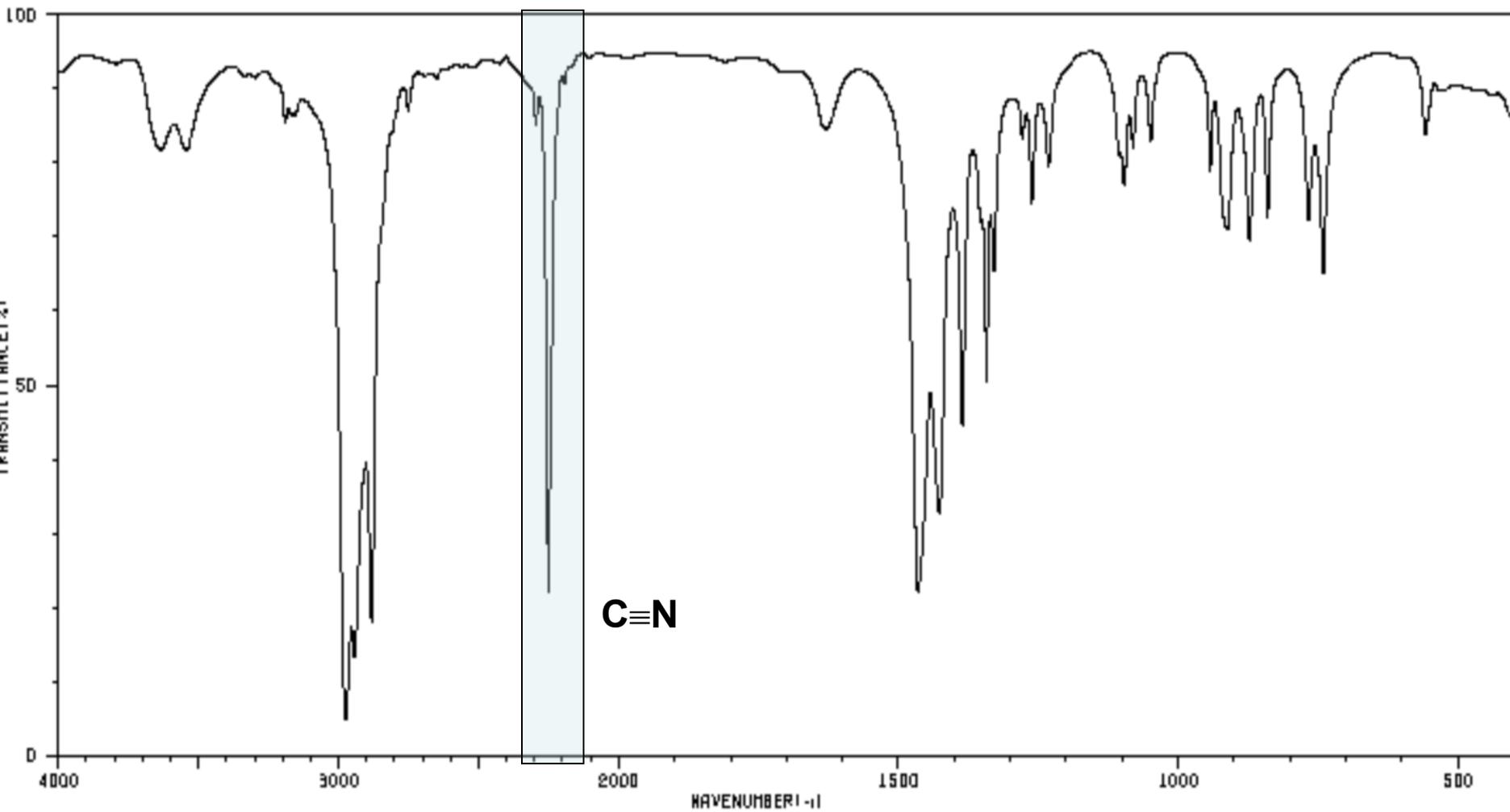
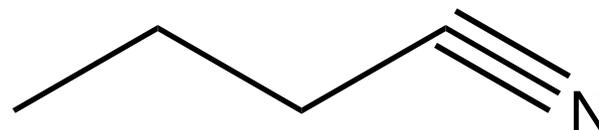


1 2 3 4 5 6 7 8

1 2 3 4 5 6 7 8

4

butanenitrile

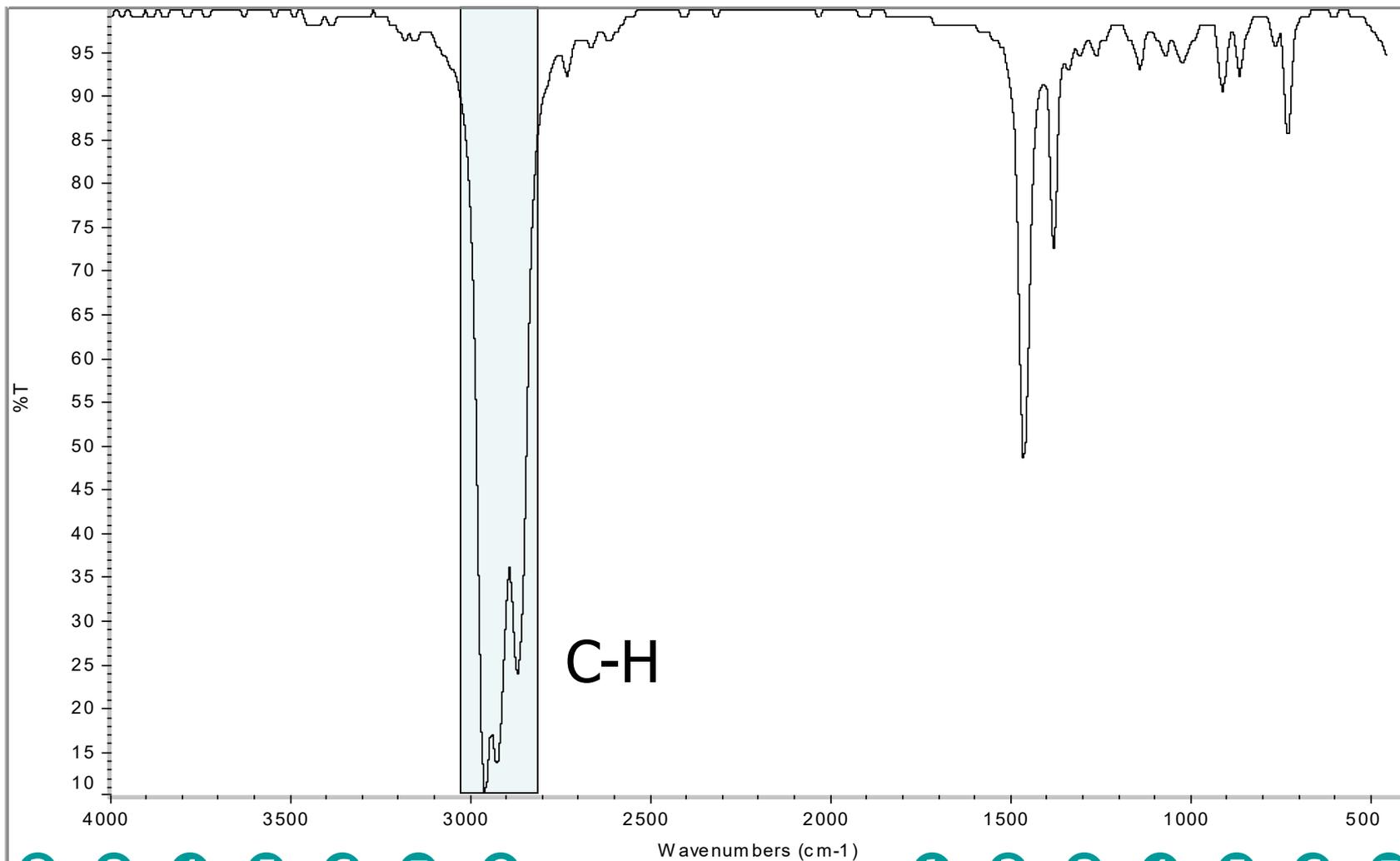


1 2 3 4 5 6 7 8

1 2 3 4 5 6 7 8

5

pentane



1

2

3

4

5

6

7

8

1

2

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4

5

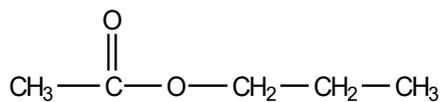
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7

8

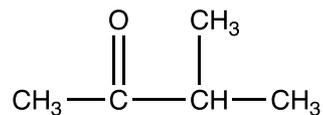
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propyl ethanoate



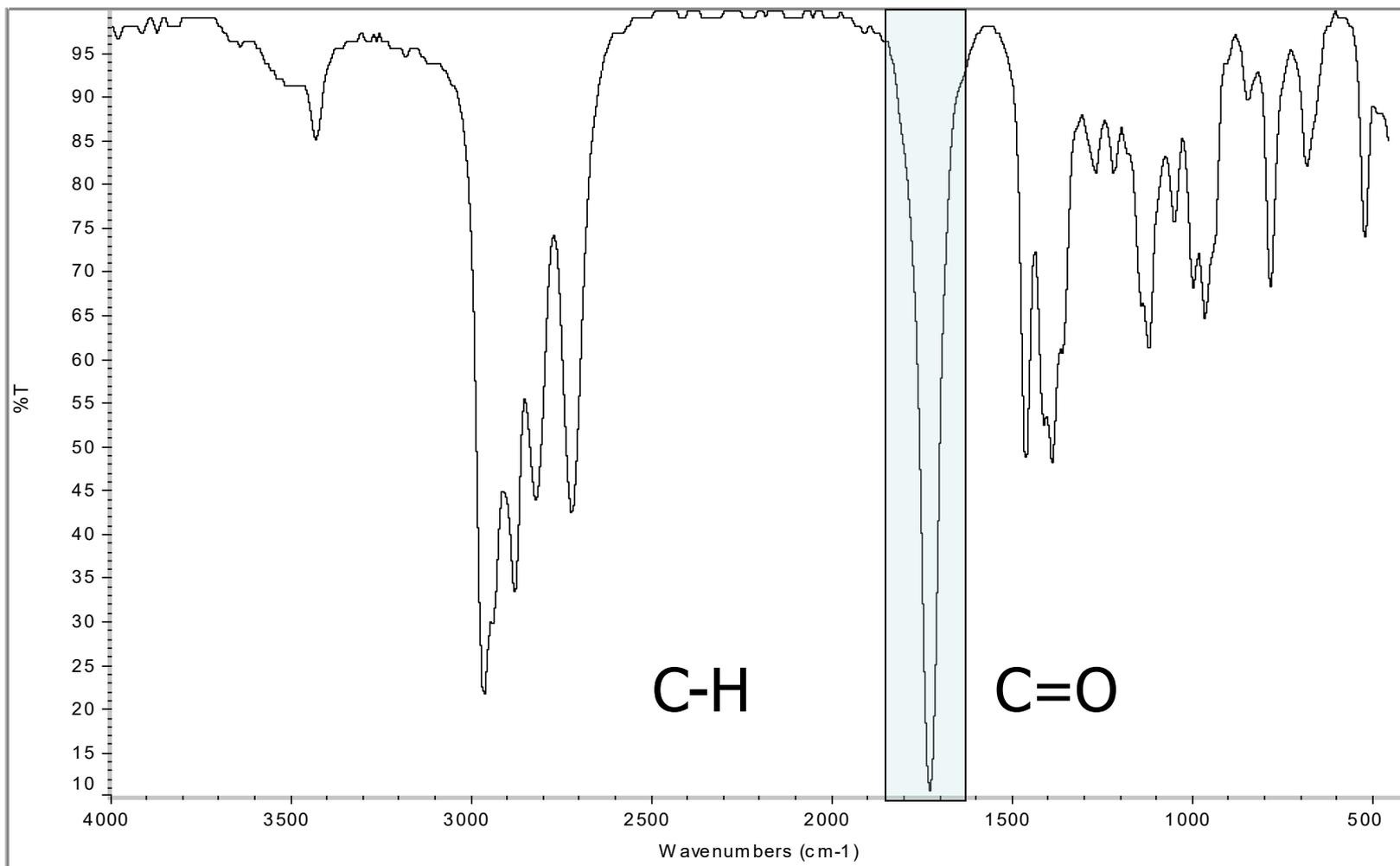
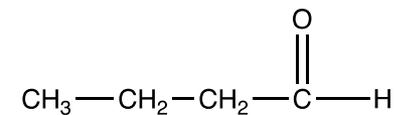
OR

2-methylpentan-3-one



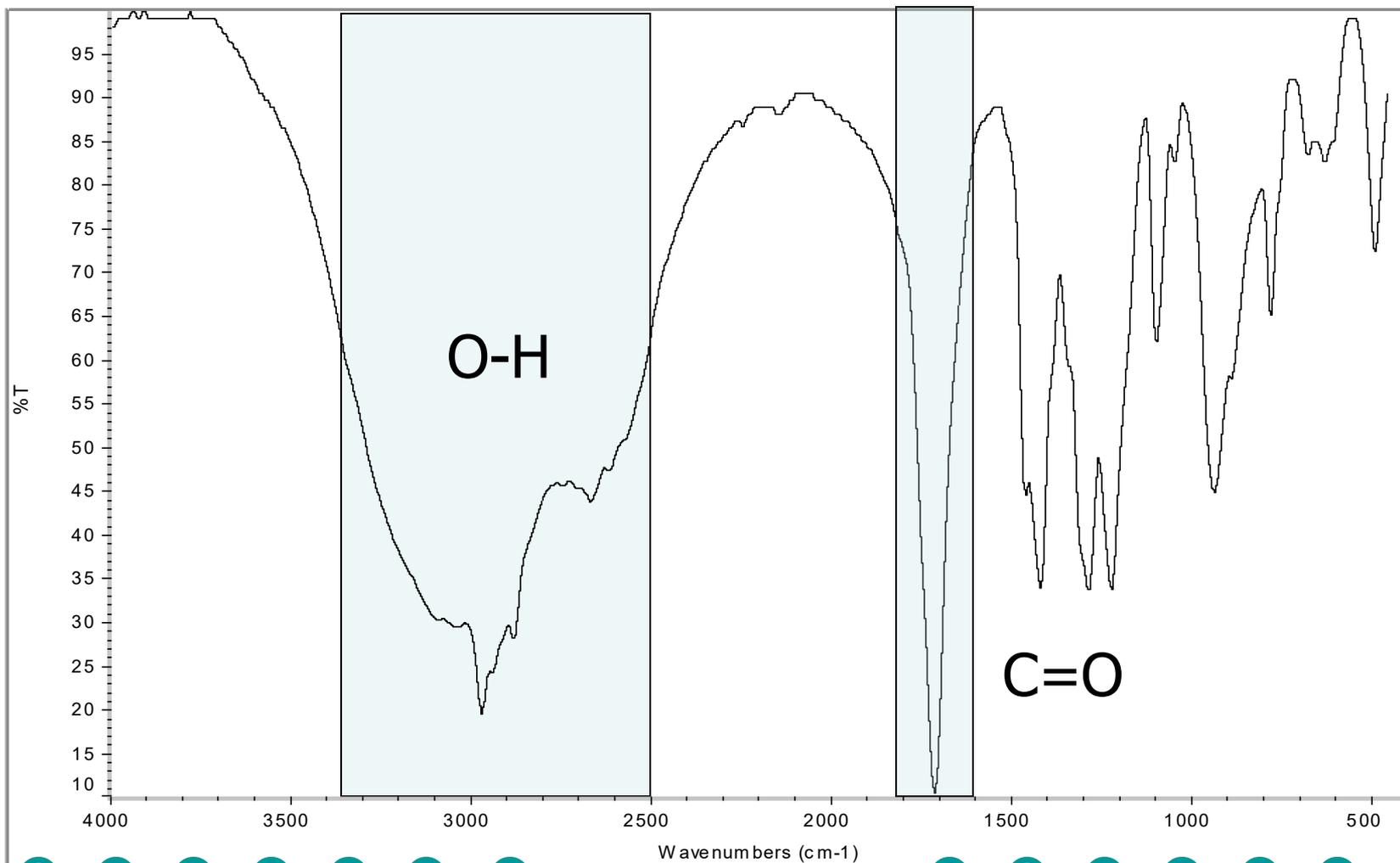
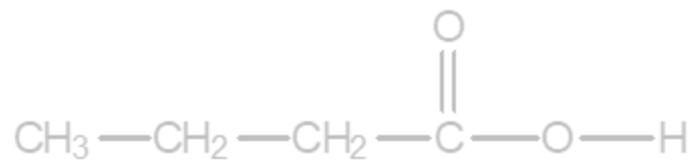
OR

butanal

**1** **2** **3** **4** **5** **6** **7** **8****1** **2** **3** **4** **5** **6** **7** **8**

7

butanoic acid

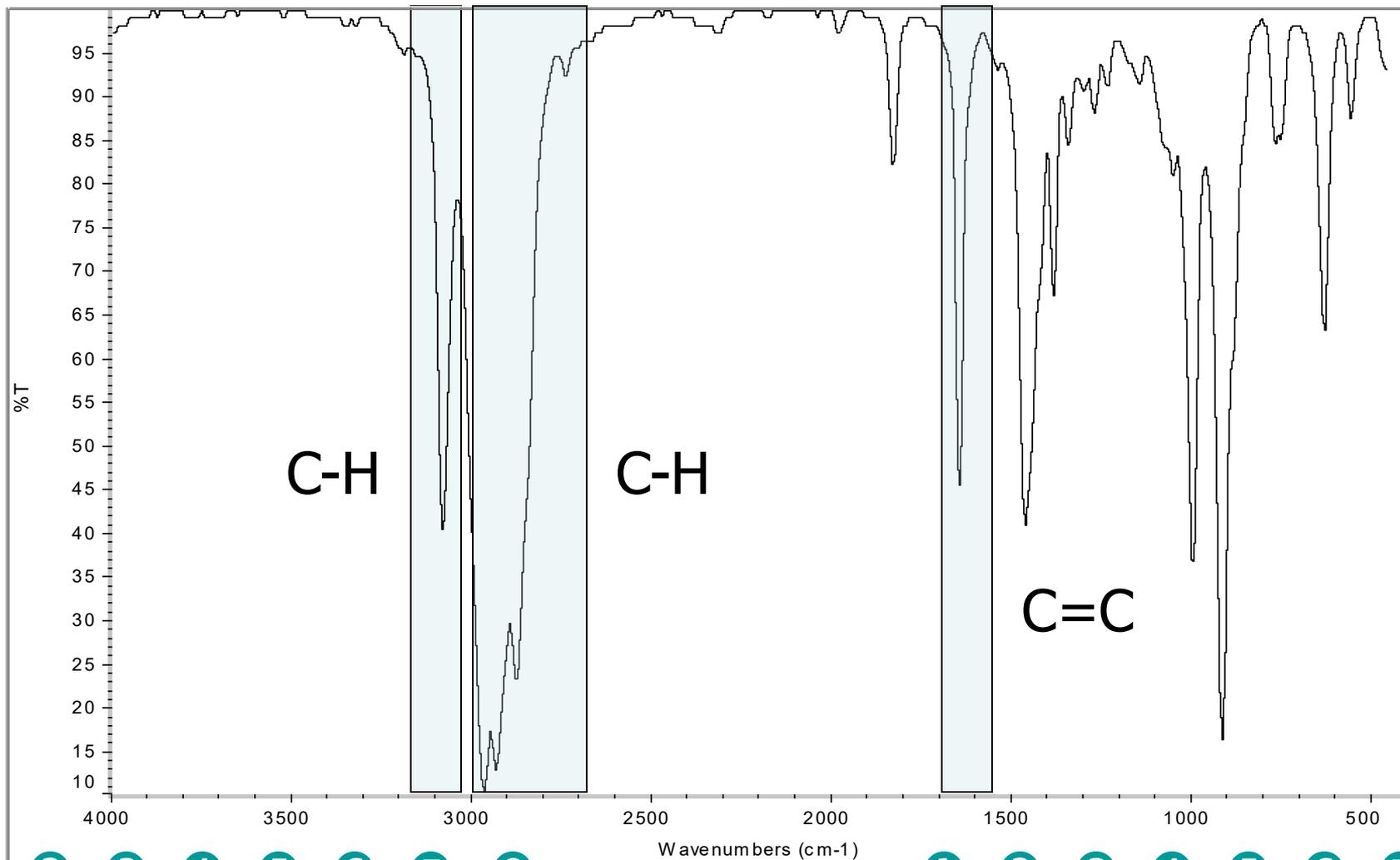


1 2 3 4 5 6 7 8

1 2 3 4 5 6 7 8

8

hex-2-ene



1

2

3

4

5

6

7

8

1

2

3

4

5

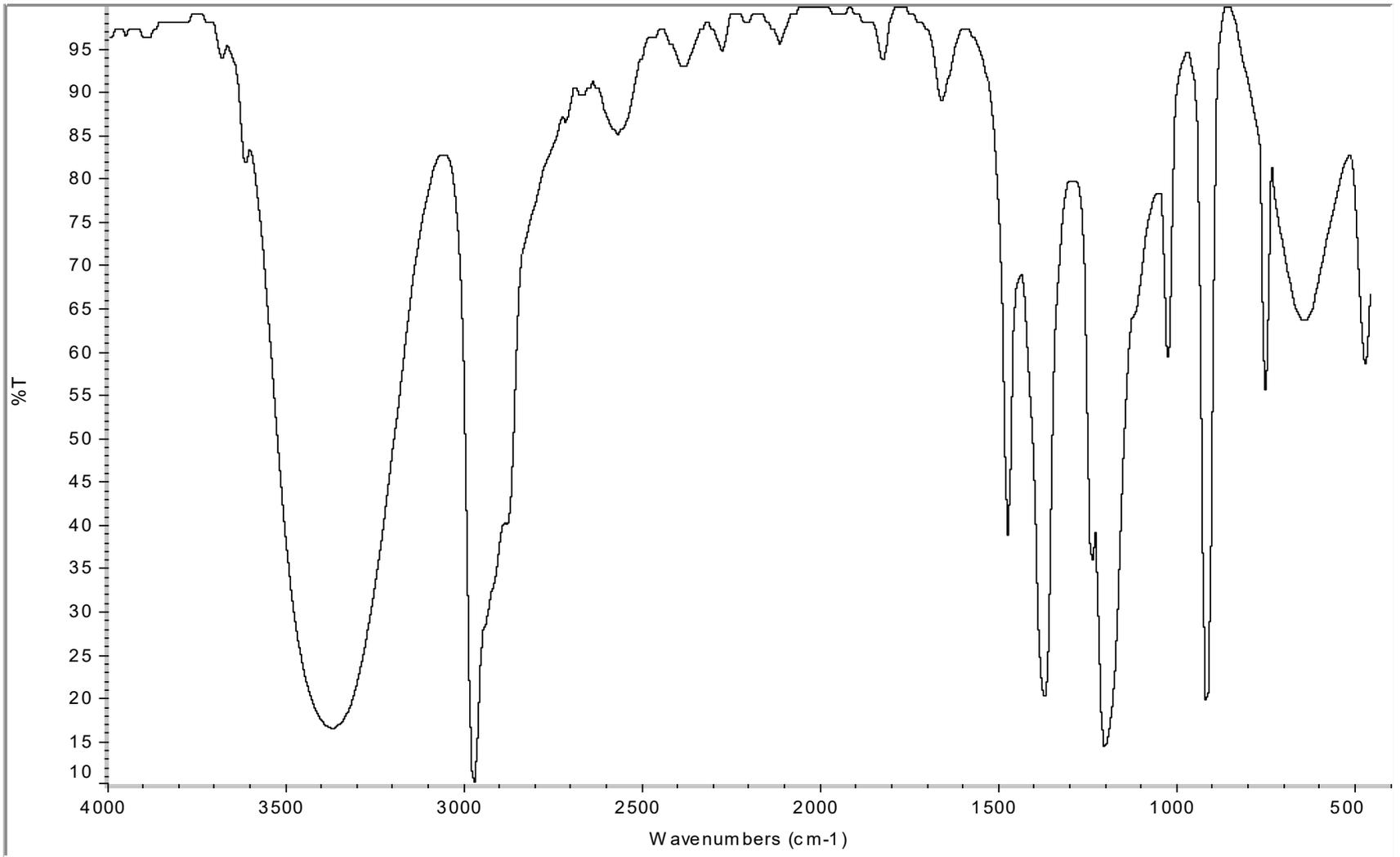
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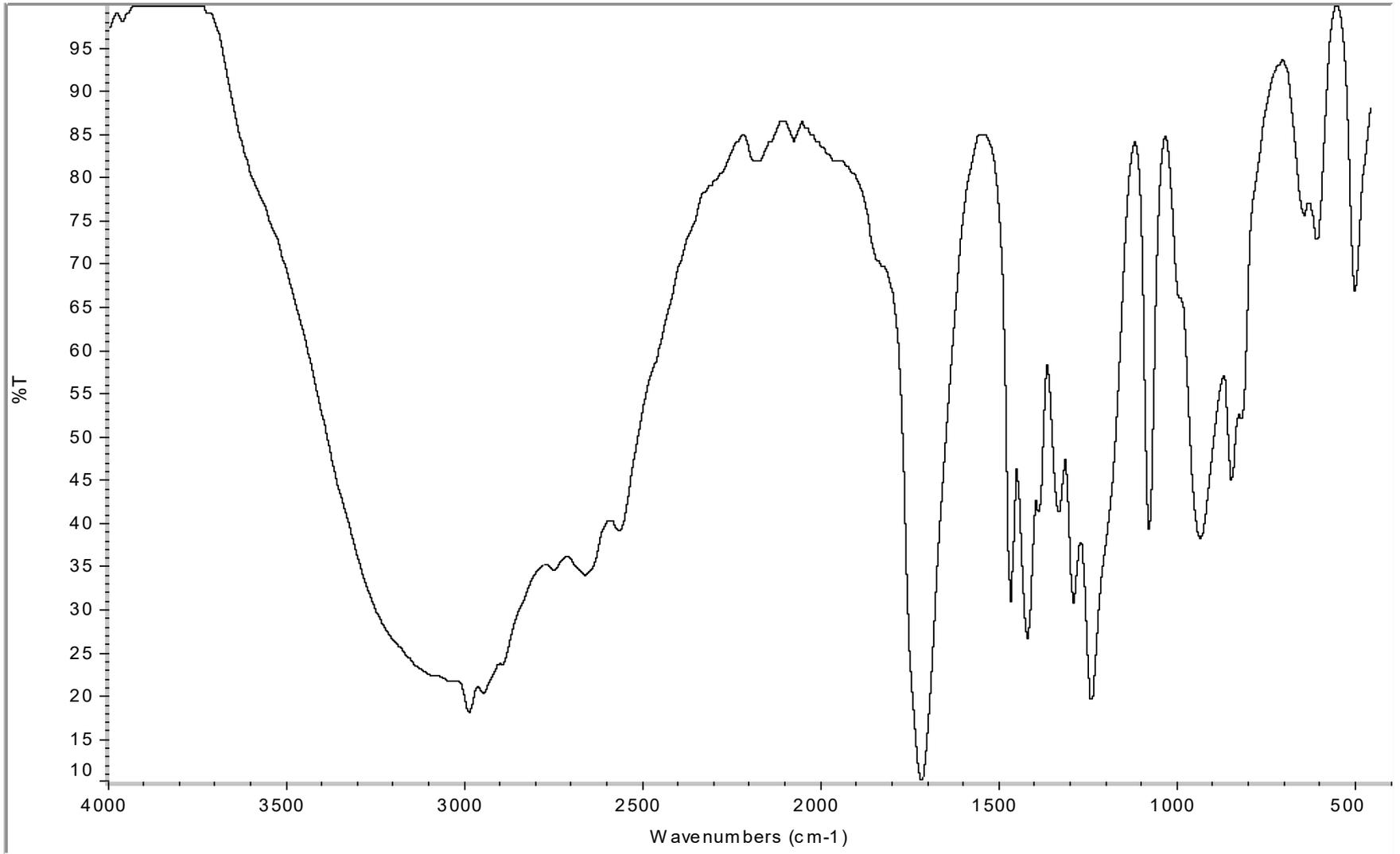
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IR Problems F/4

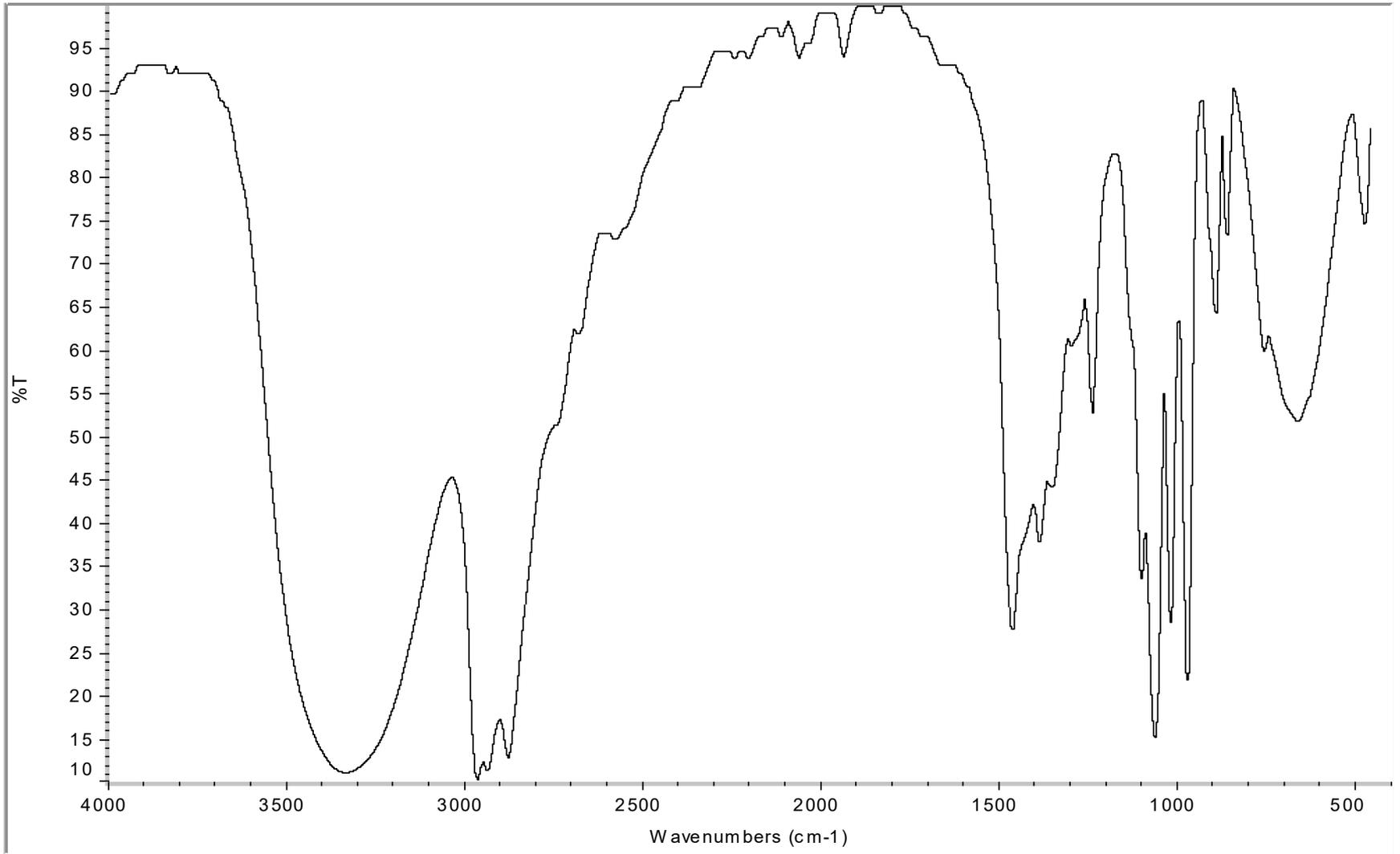
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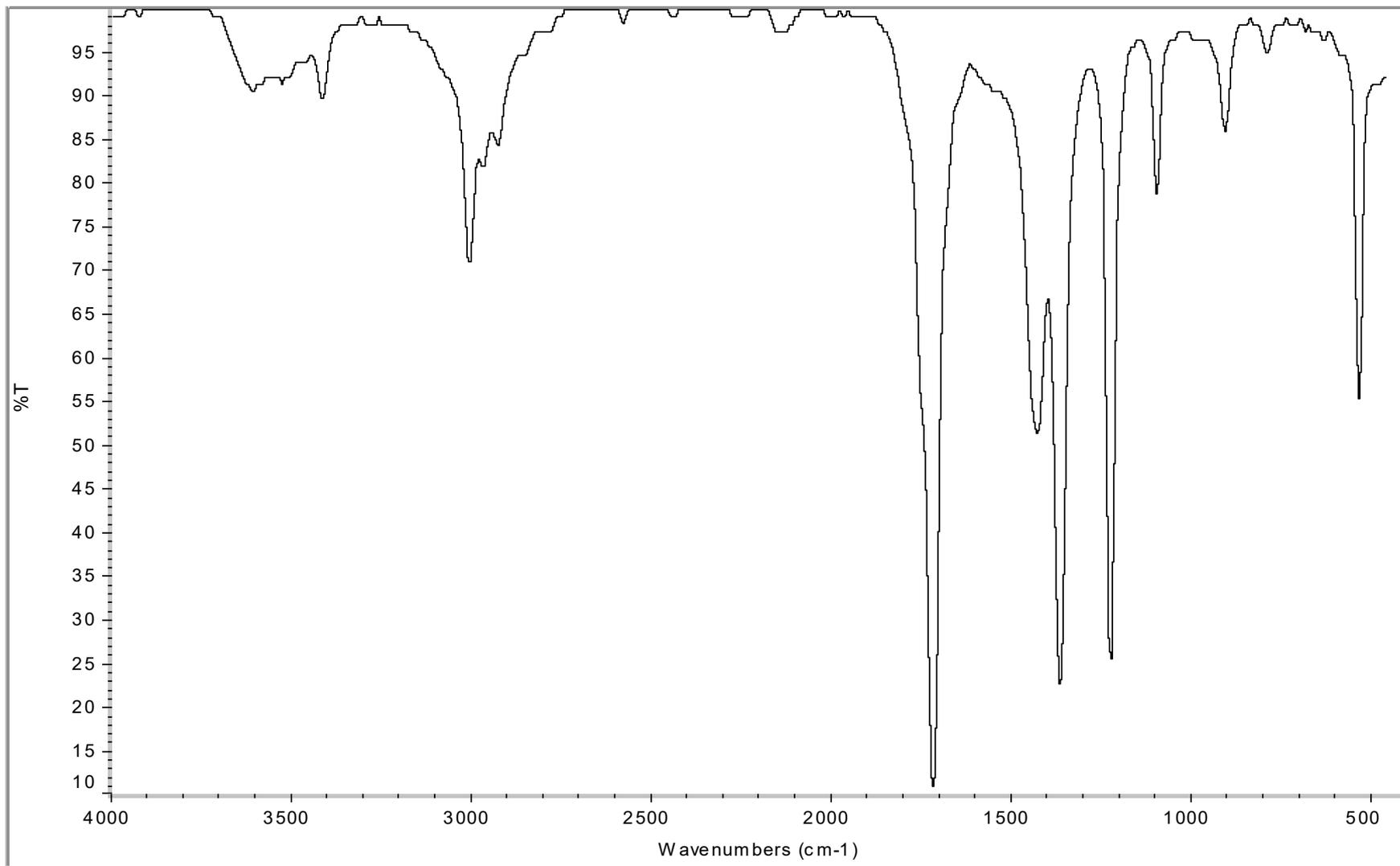
G



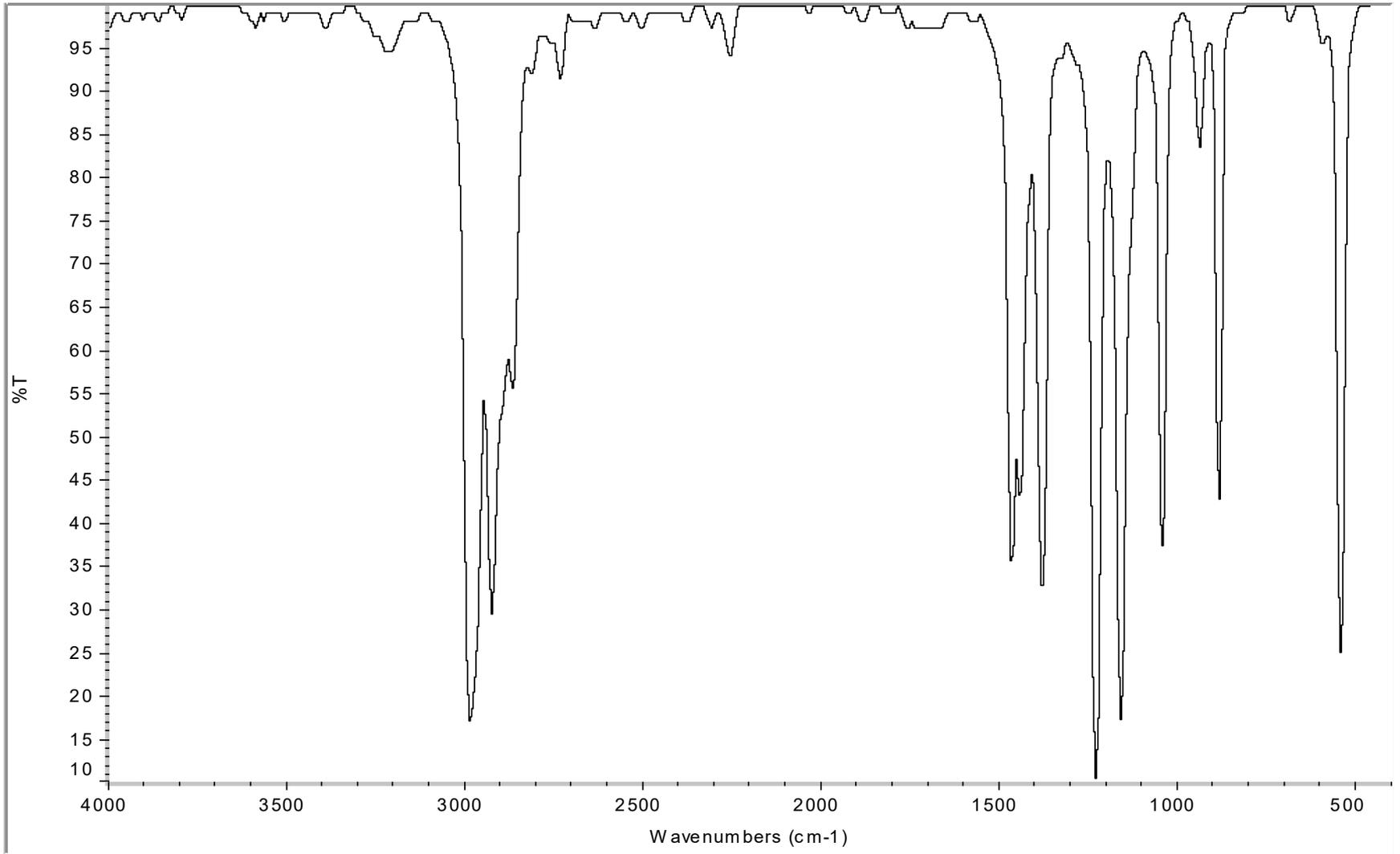
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2



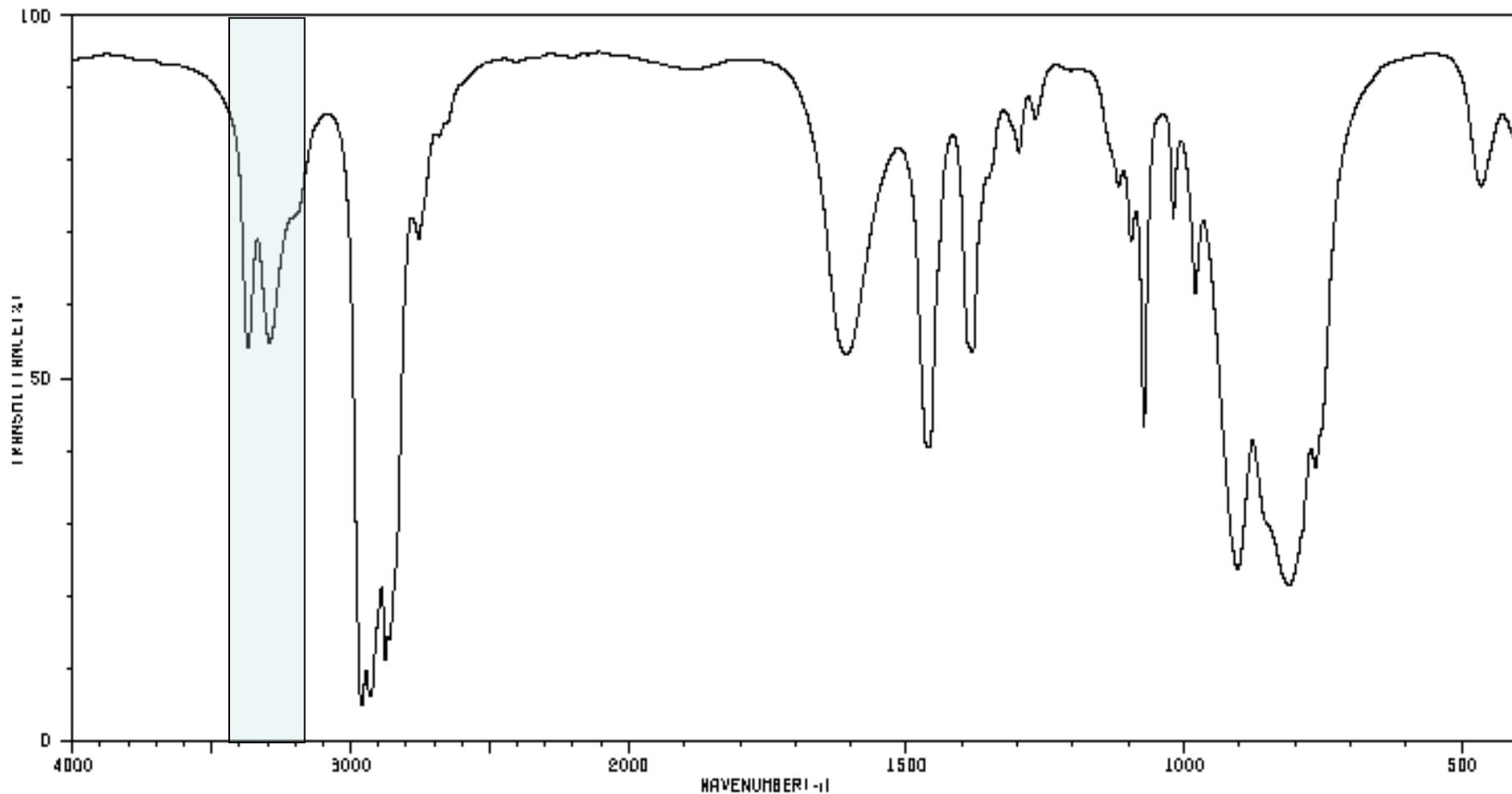
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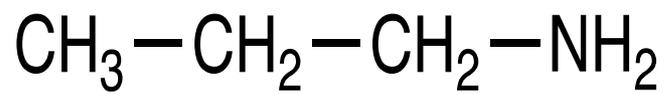
Most IR spectra are from the SBDS data base

IR Problems B/5

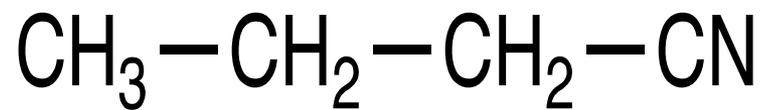
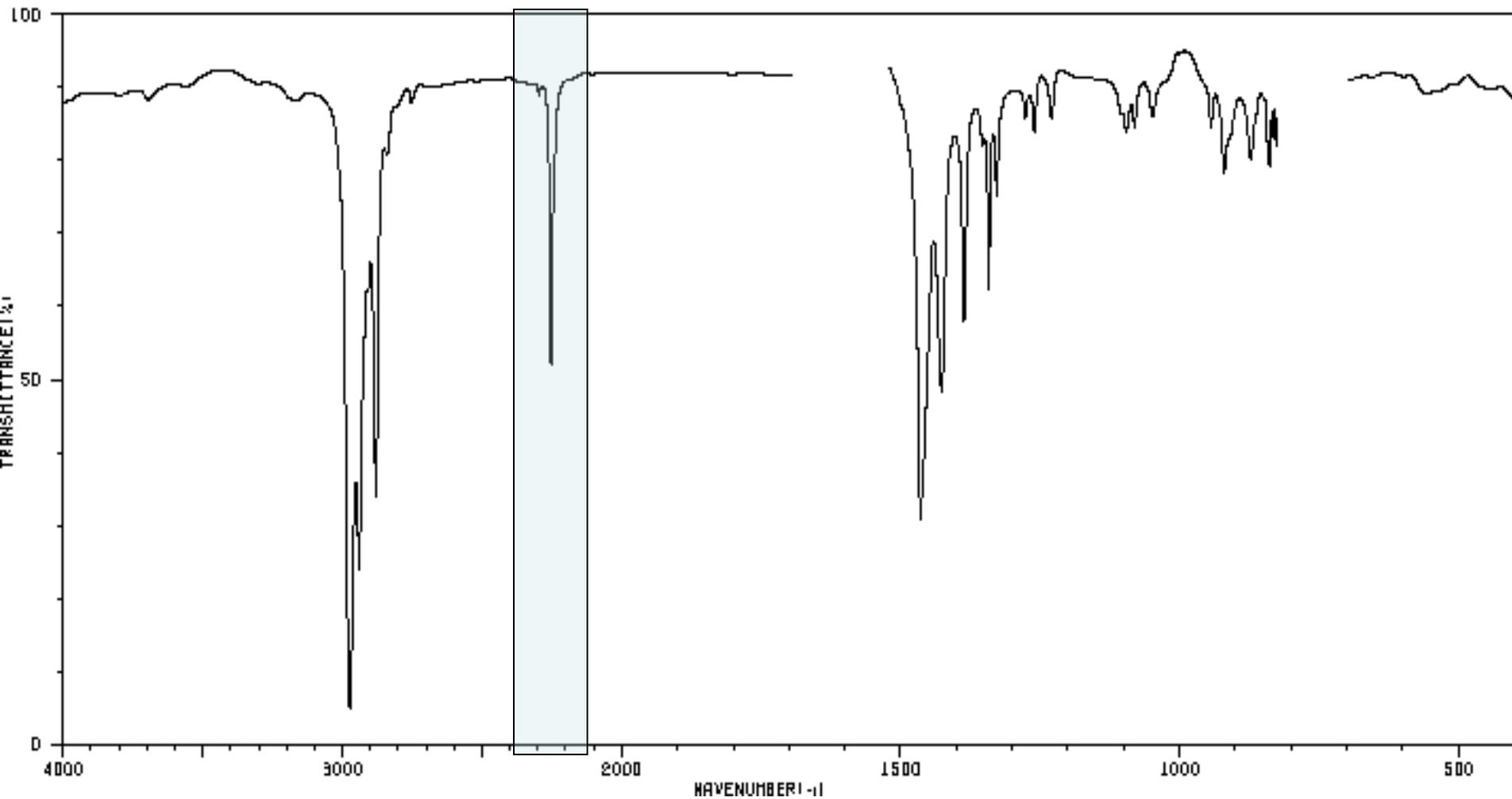
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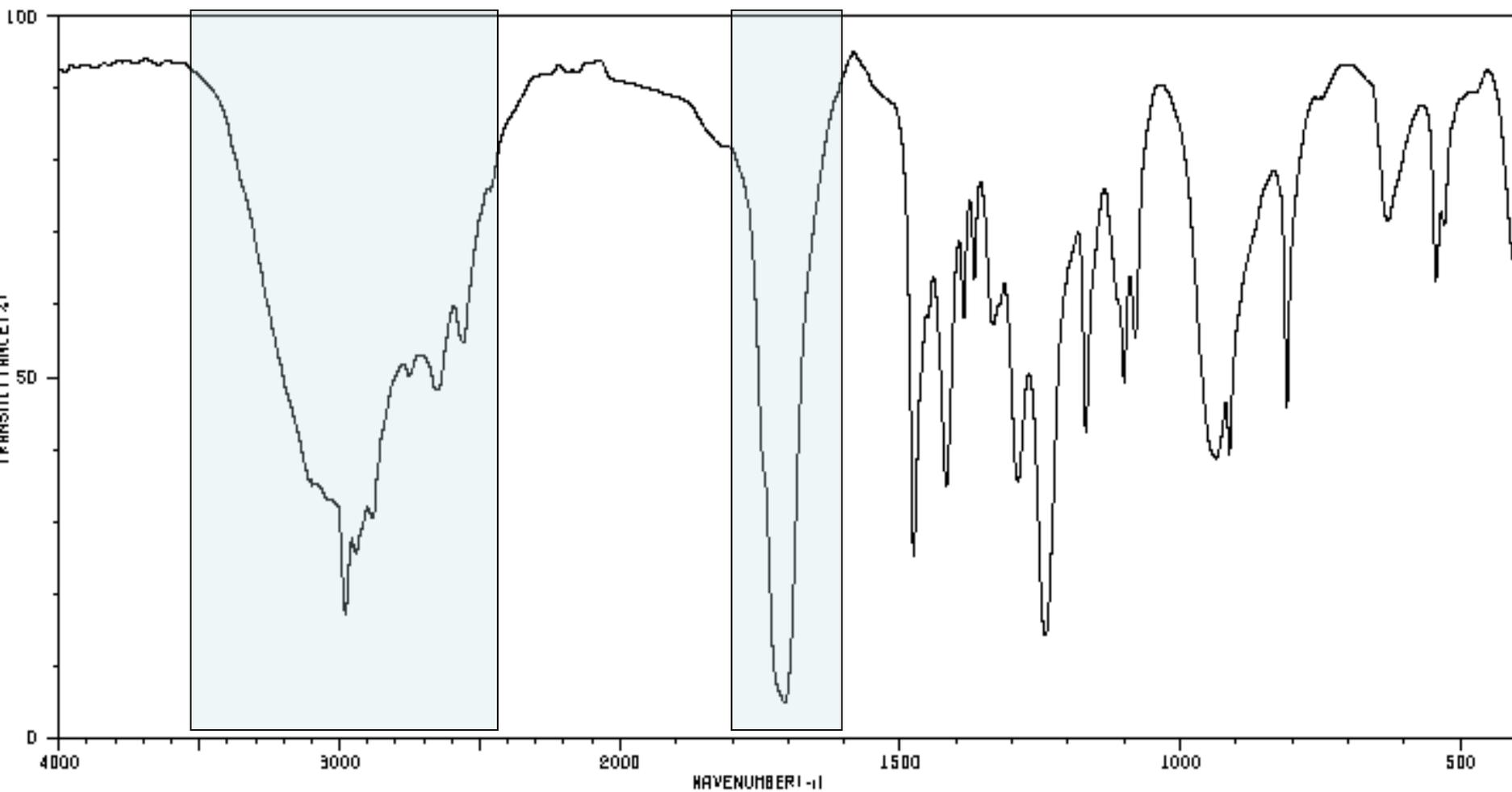
N-H



2

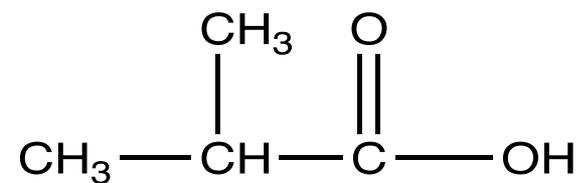


3

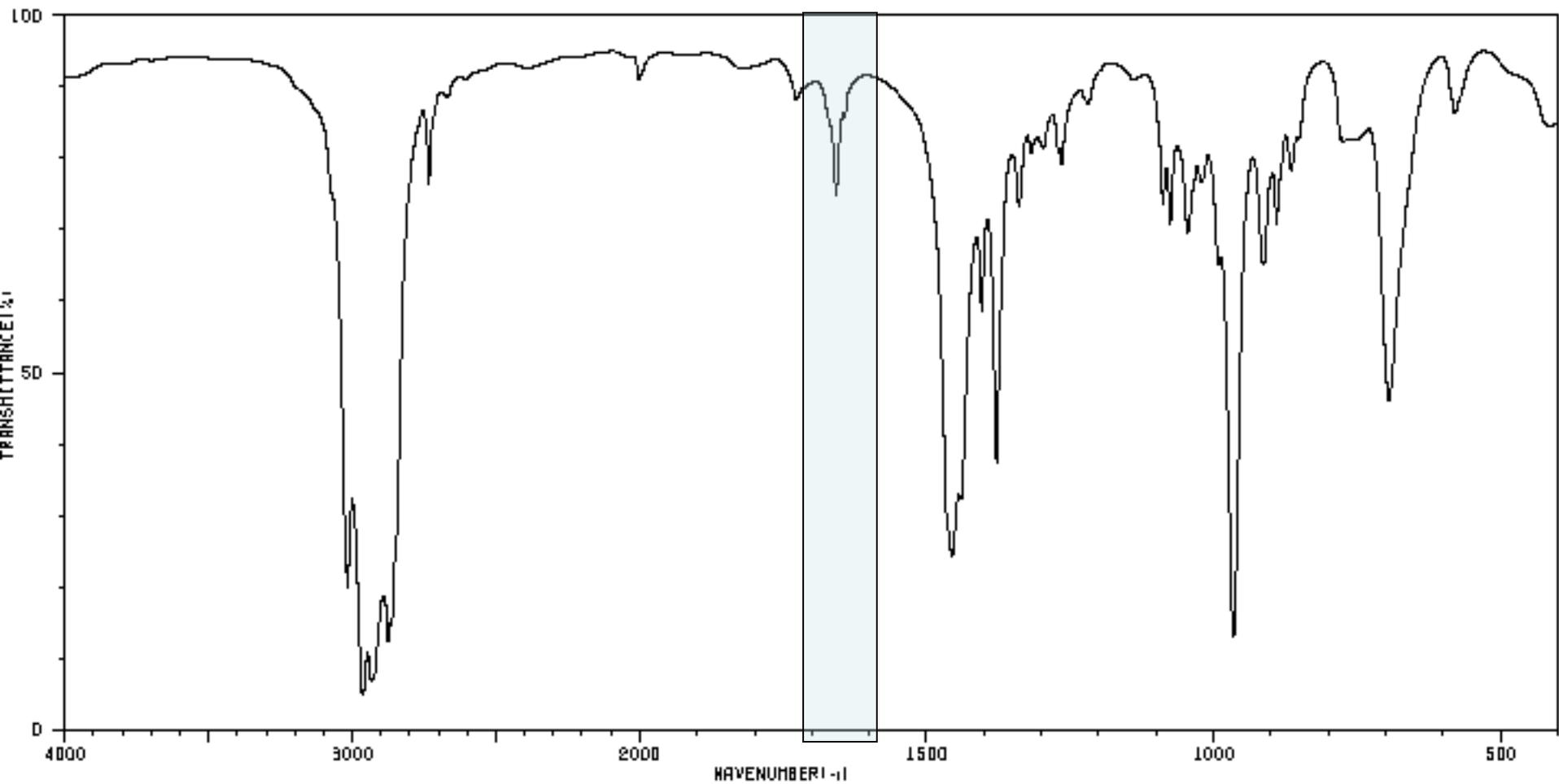


Acid O-H

C=O



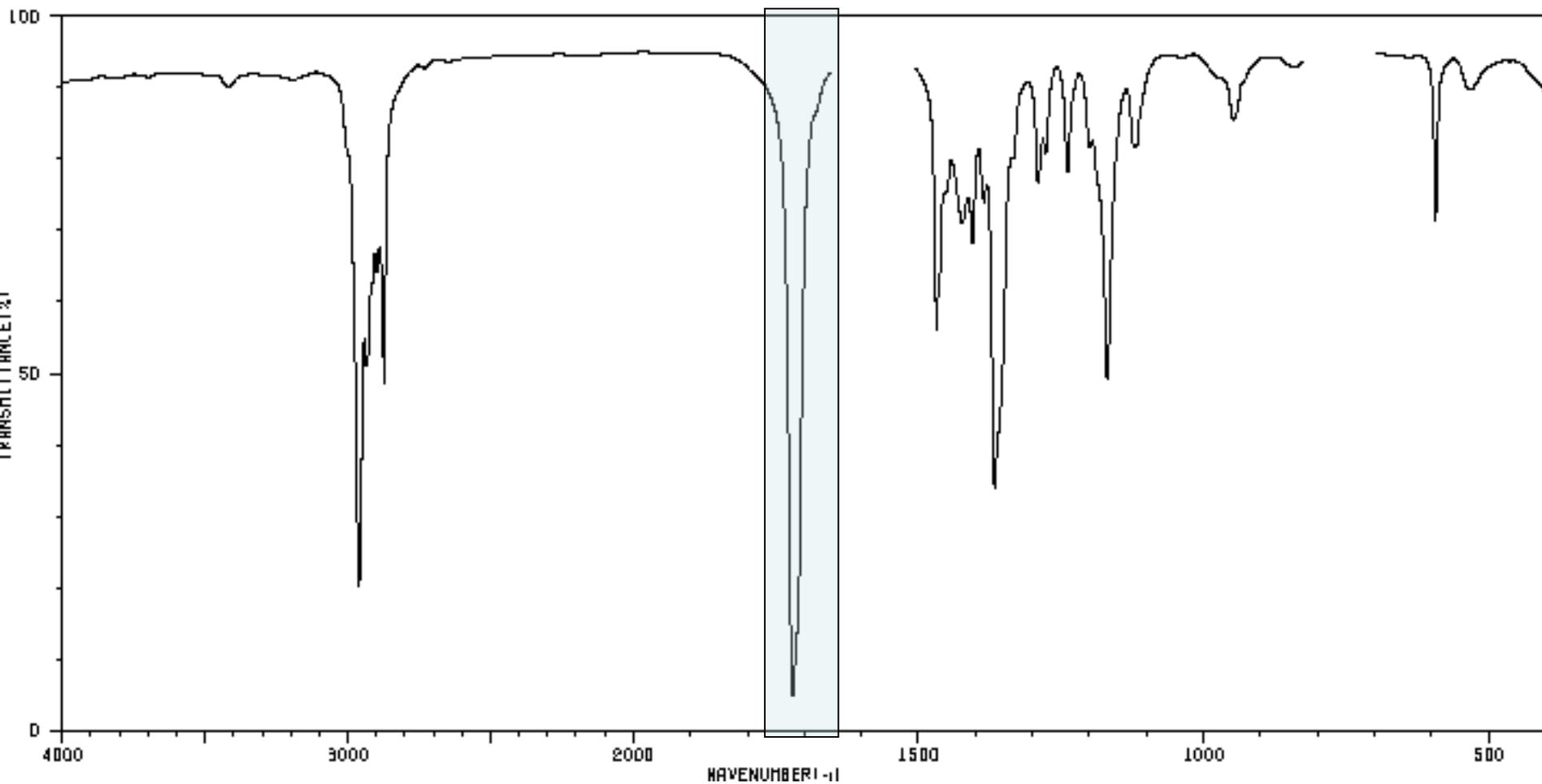
4



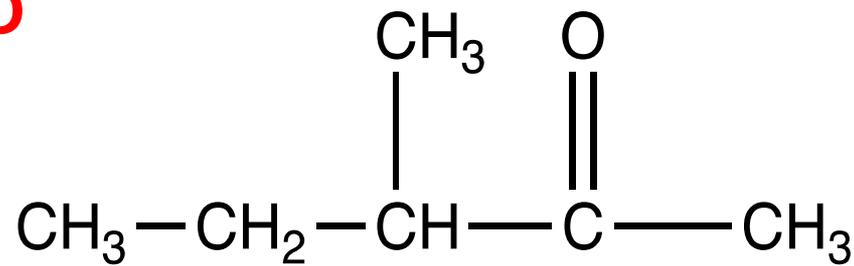
C=C



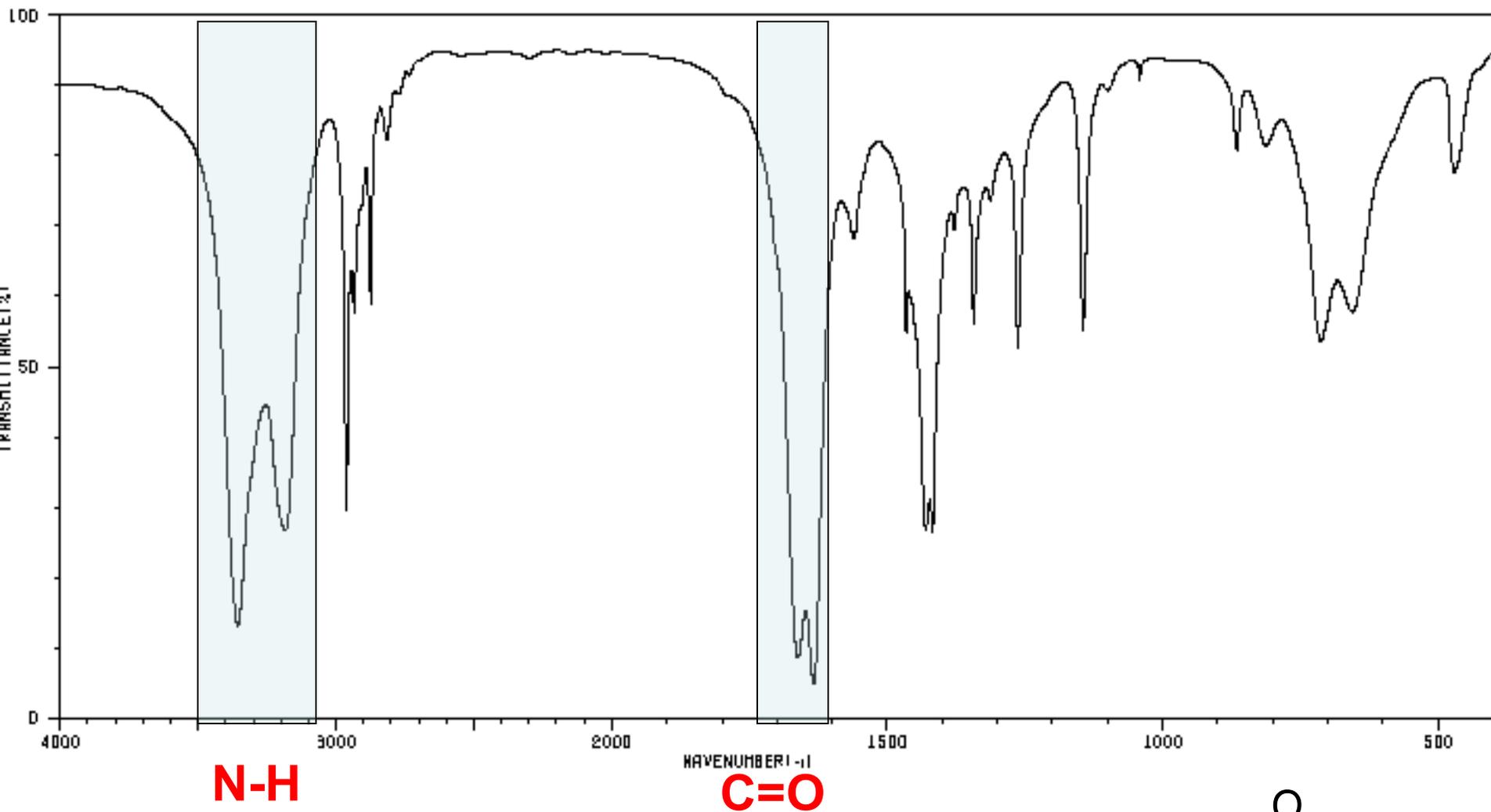
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C=O

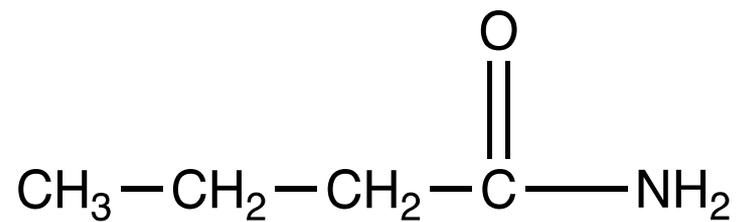


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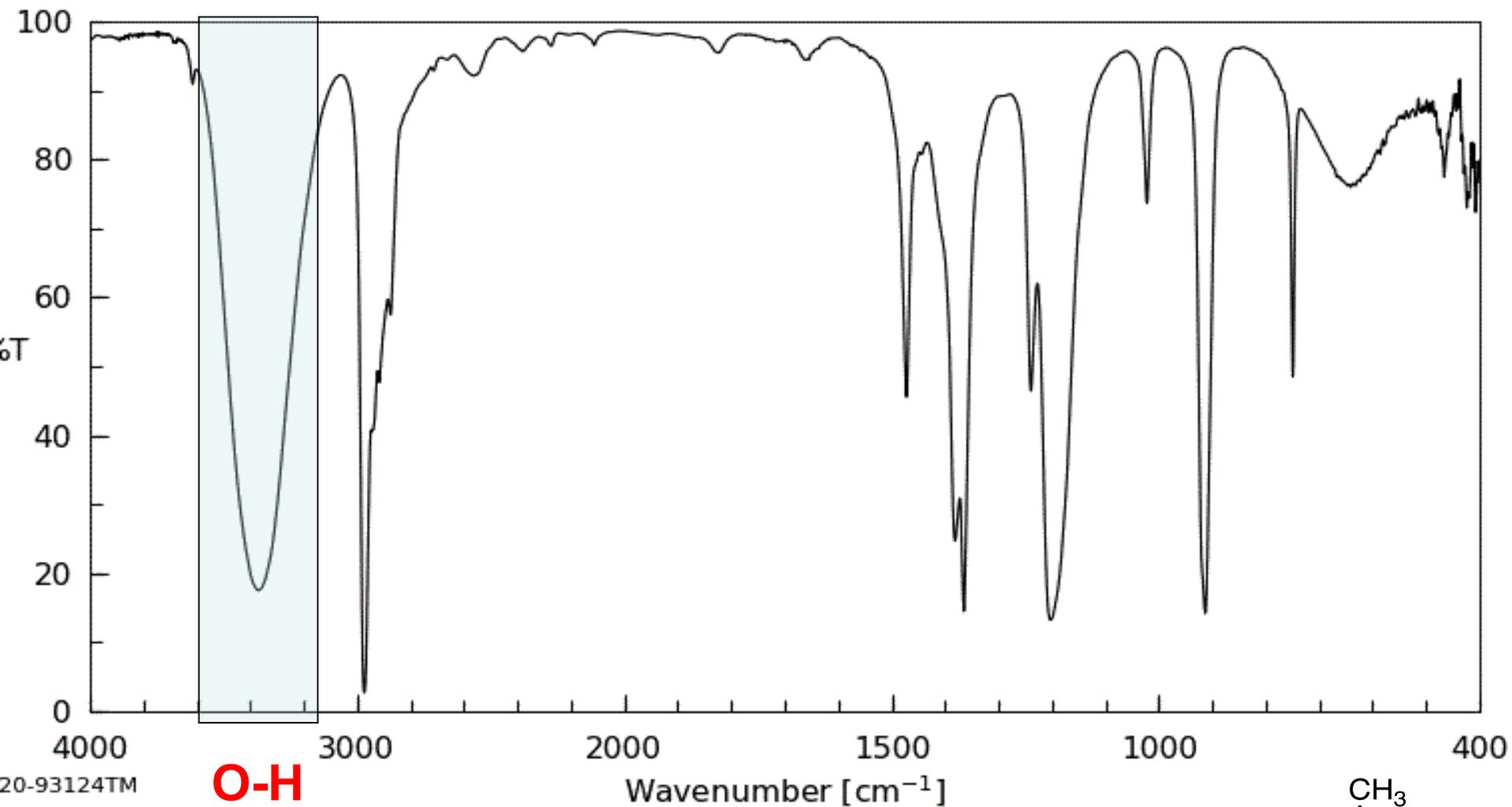


N-H

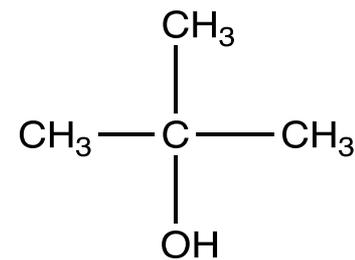
C=O



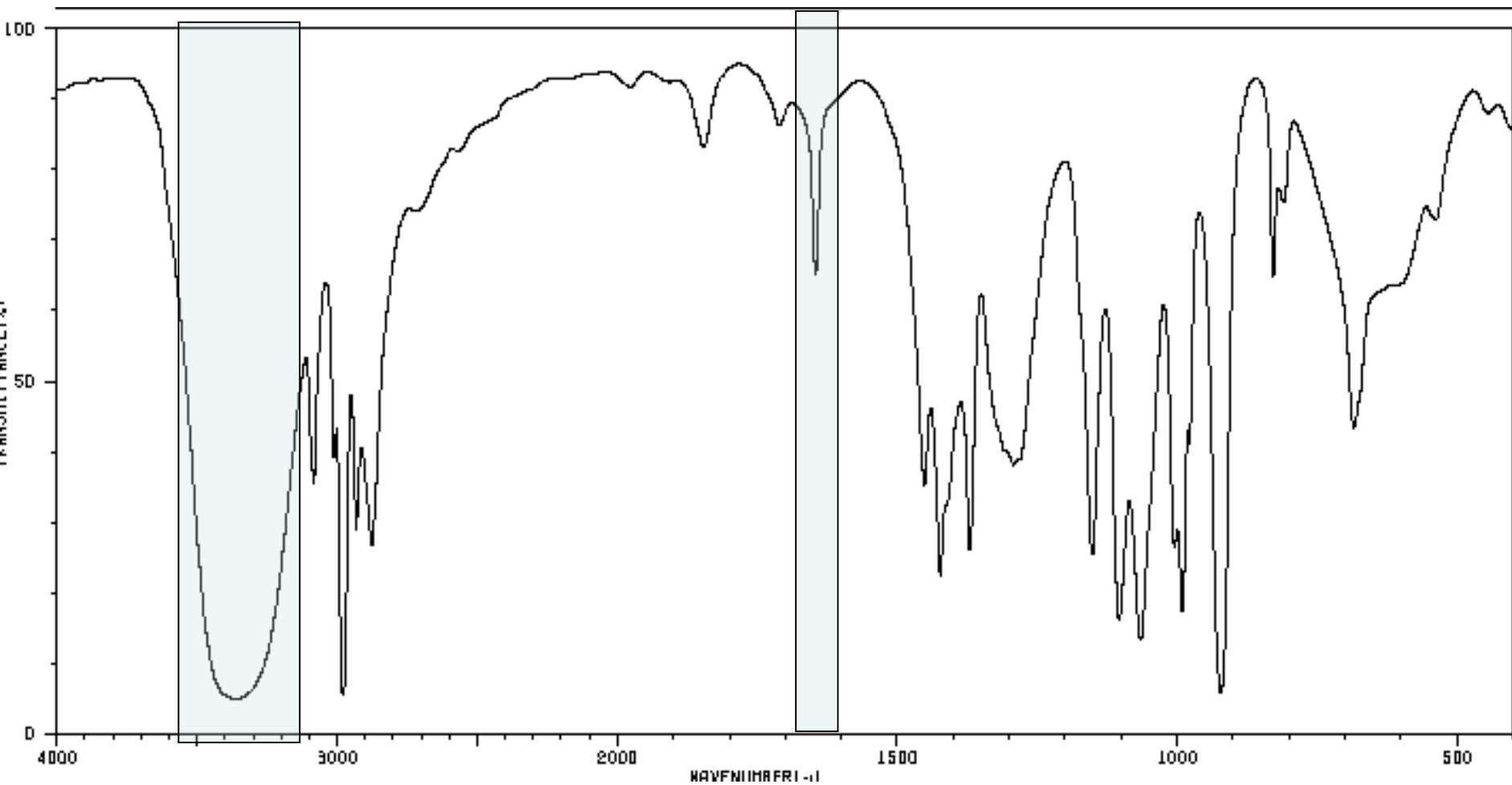
7



O-H
alcohol



8



O-H
alcohol

C=C

