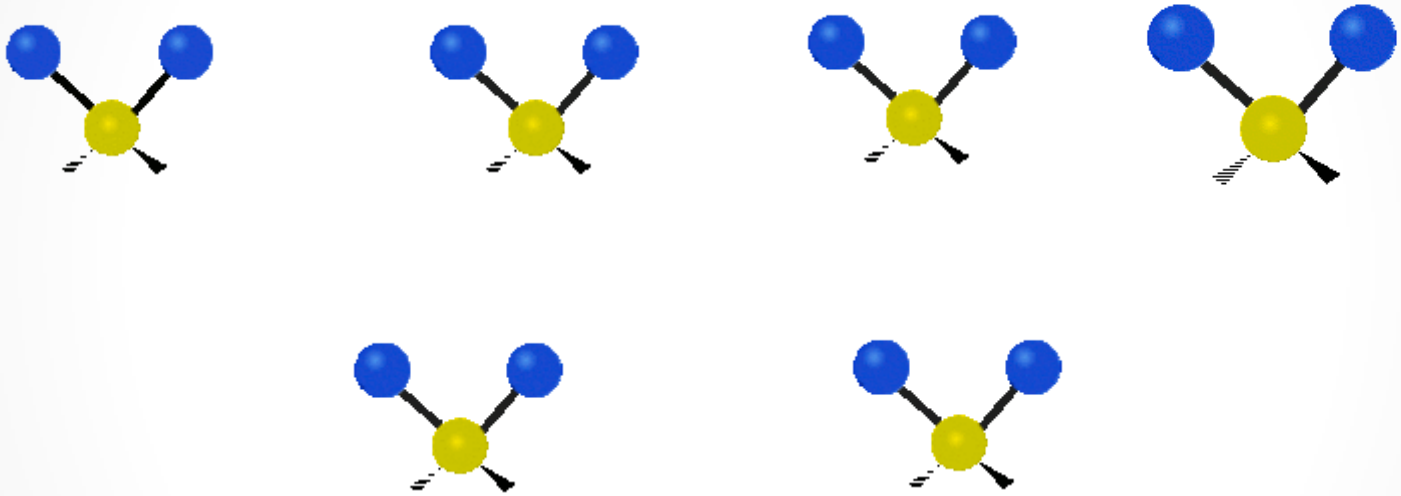
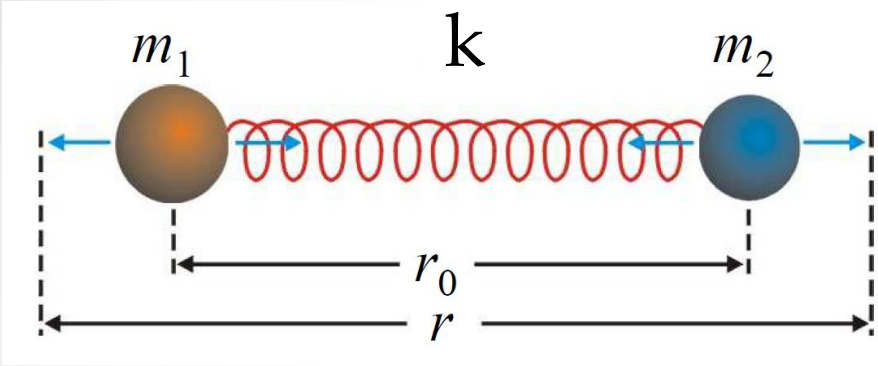
IR – spectroscopy part I

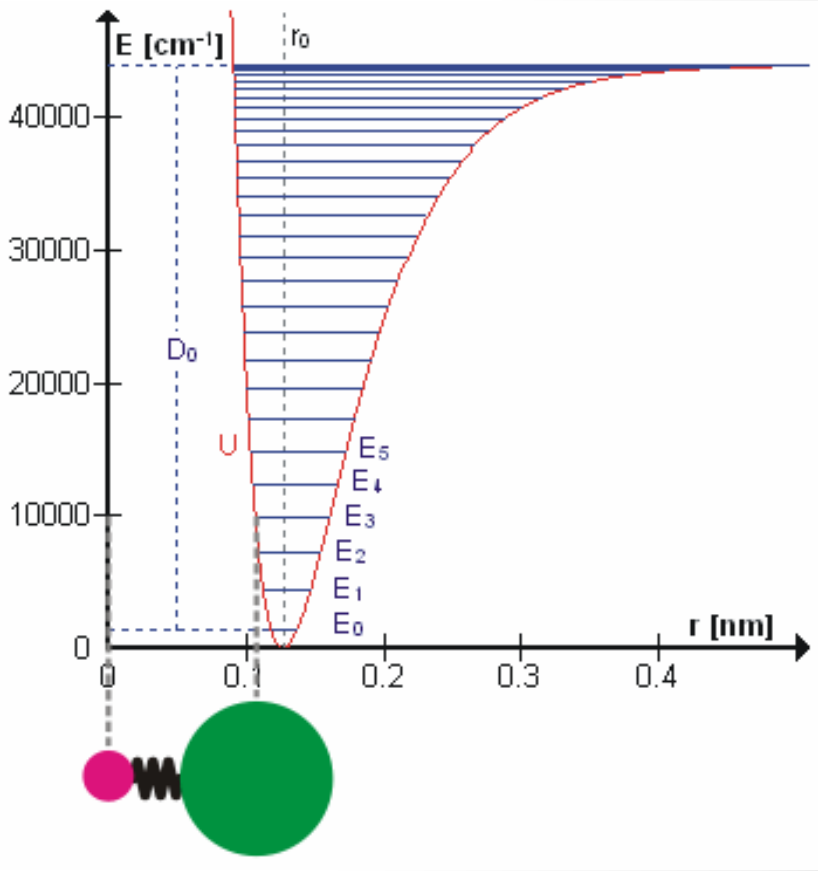


Mechanical oscillator -

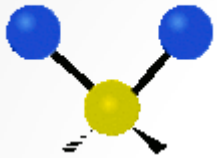
„two atoms and chemical bond”



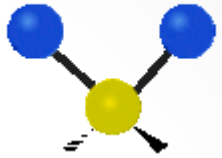
$$F = -kq$$



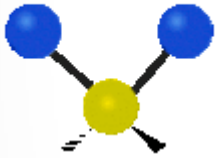
Vibrational modes for CH_2



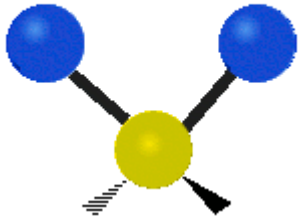
Symmetrical streching ν_s



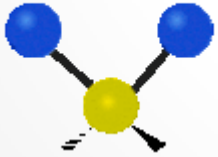
Asymmetrical streching ν_{as}



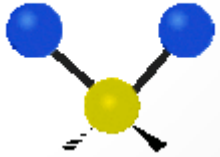
In-plane scissoring δ_s



In-plane bending ρ



Out-of-plane bending (wagging) ω

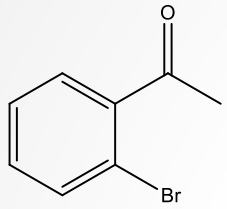


Out-of-plane bending (twisting) τ

Electromagnetic spectrum

Spectral region	VHF	UHF	Microwave	Infrared	Visible	Ultraviolet	X-rays	γ-rays
Common usage	NMR	EPR	rotational transitions	vibrational transitions	electronic transitions		ionisation	nuclear effects
Frequency (Hz)	5×10^{8}	3×10^{10}	3×10^{11}	3×10^{13}	6×10^{14}	1.2×10^{15}	3.0×10^{17}	1.5×10^{19}
Wavelength	0.6 m	1 cm	1 mm	10 μm	500 nm	250 nm	1 nm	20 pm
Wavenumber (cm^{-1})	0.017	1.0	10.0	1000	20,000	40,000	1.0×10^{7}	5.0×10^{8}
Single photon energy (eV)	2.07×10^{-6}	1.24×10^{-4}	1.24×10^{-3}	1.24×10^{-1}	2.5	5.0	1.24×10^{3}	6.2×10^{4}
Photon energy ($kJ\ mol^{-1}$)	2.03×10^{-4}	1.20×10^{-2}	1.20×10^{-1}	12.0	239	479	1.2×10^{5}	6×10^{6}

Appearance of IR Spectrum

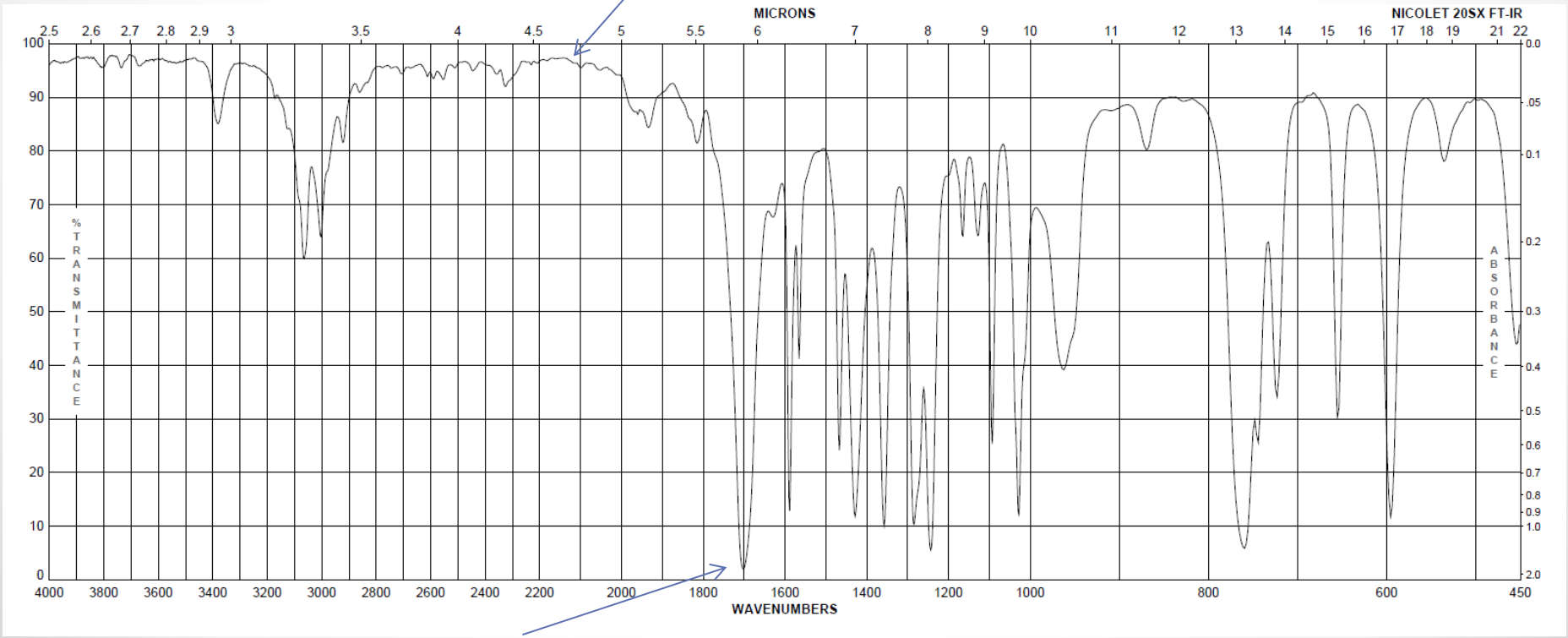


1-(2-bromophenyl)ethanone

o-bromoacetophenone

98% transmission

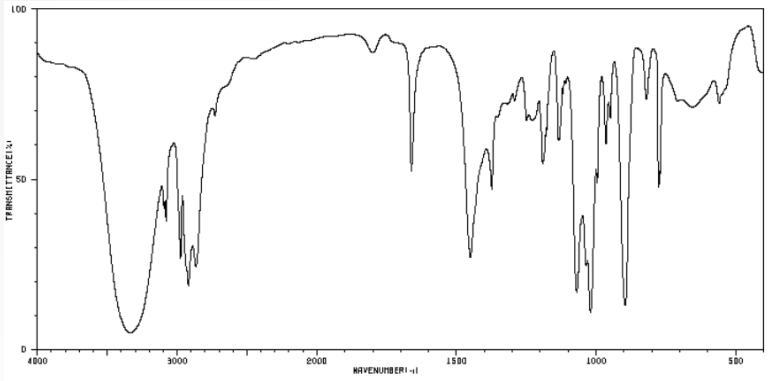
Wavelenght μ= 10^{-6} meter

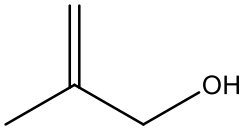


3% transmission

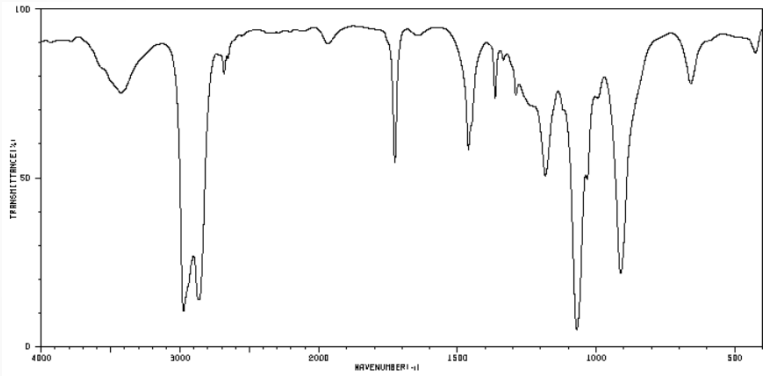
Wavenumber (frequency) cm^{-1} = Hz /c

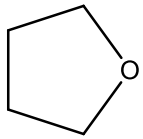
Functional isomers in IR





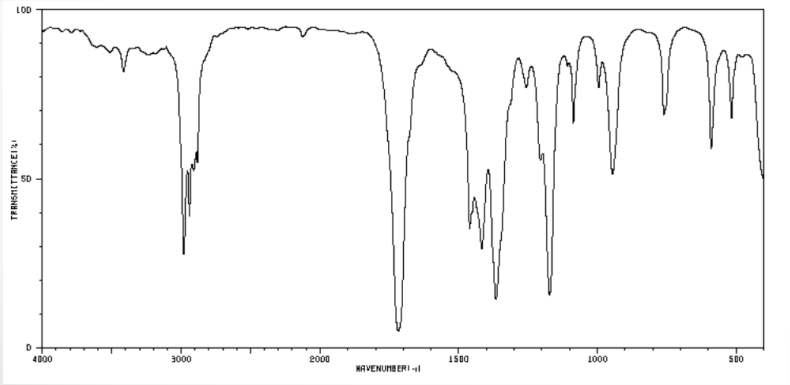
2-methylprop-2-en-1-ol

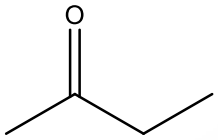




tetrahydrofuran

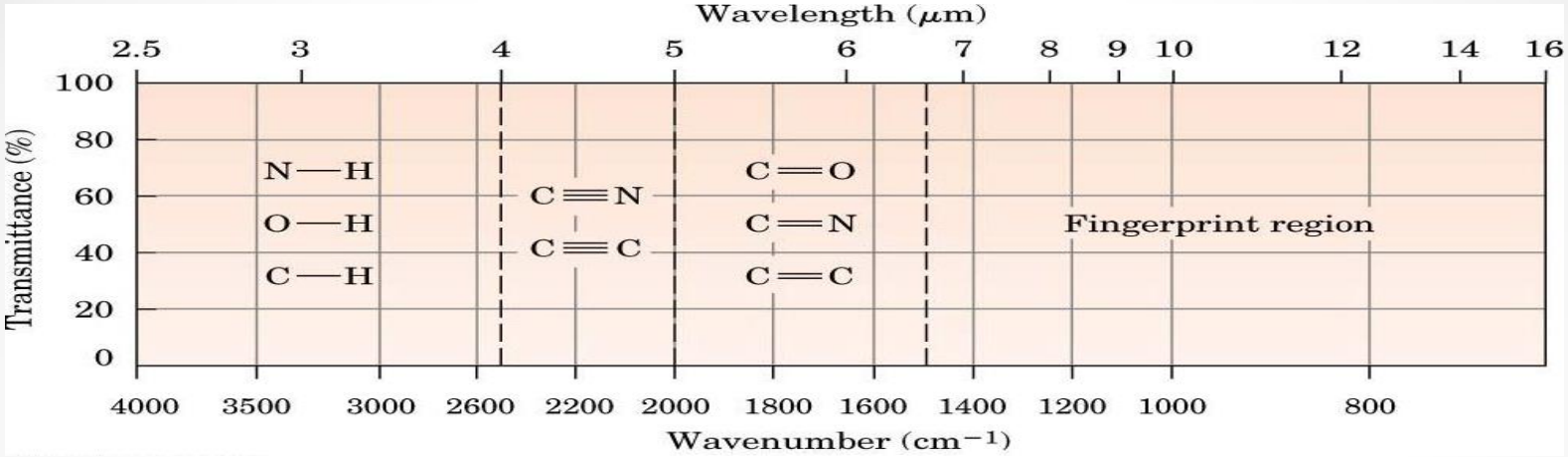
C_4H_8O

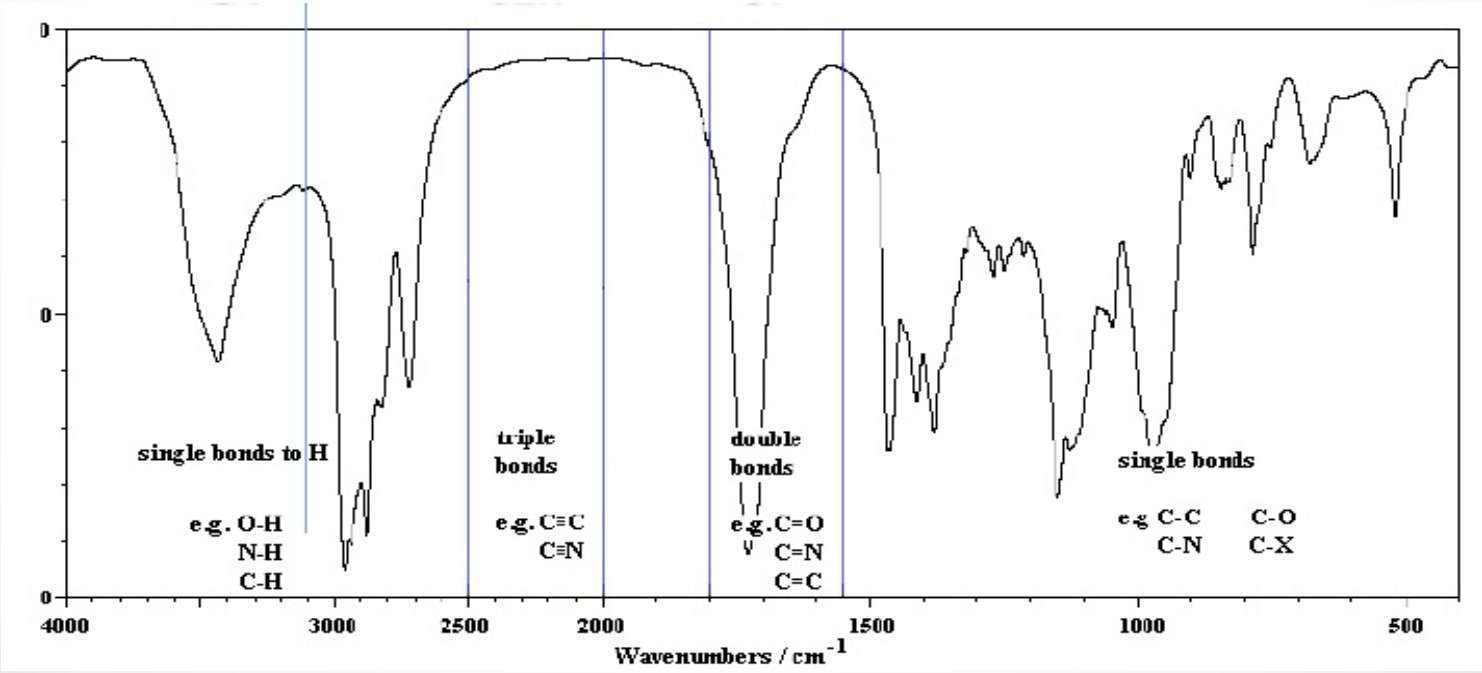




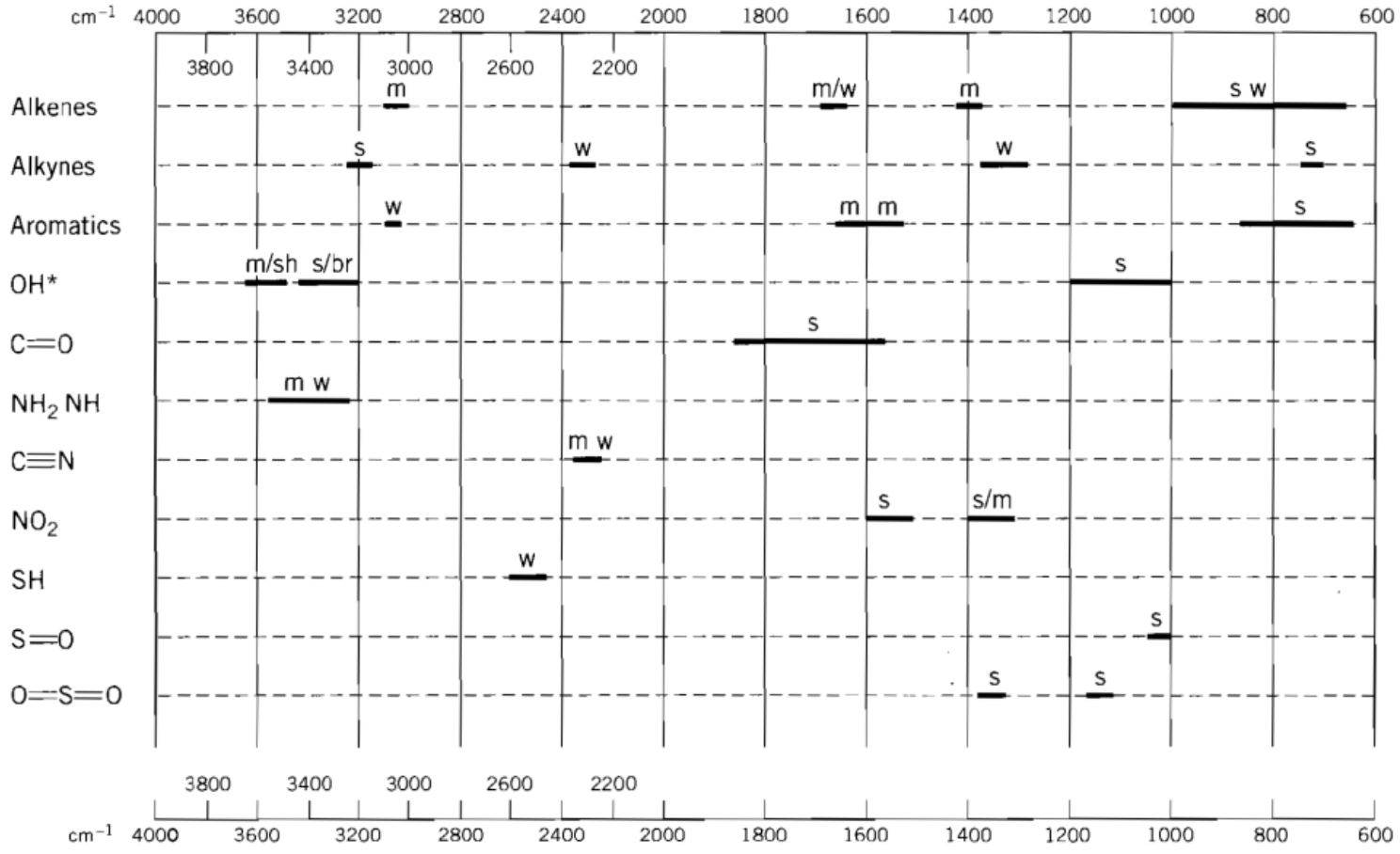
butan-2-one

Regions of the IR spectrum



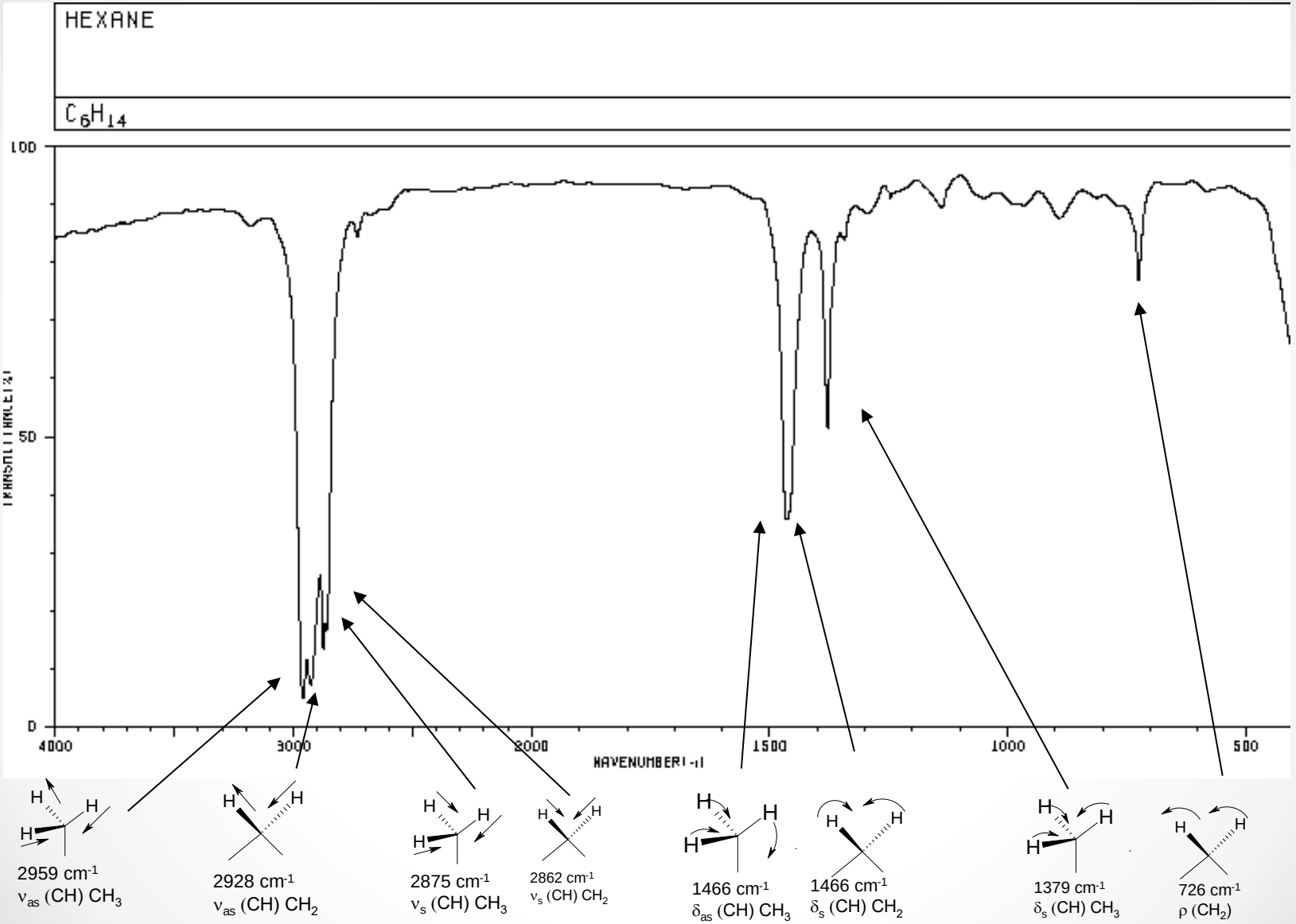


Regions of the IR spectrum

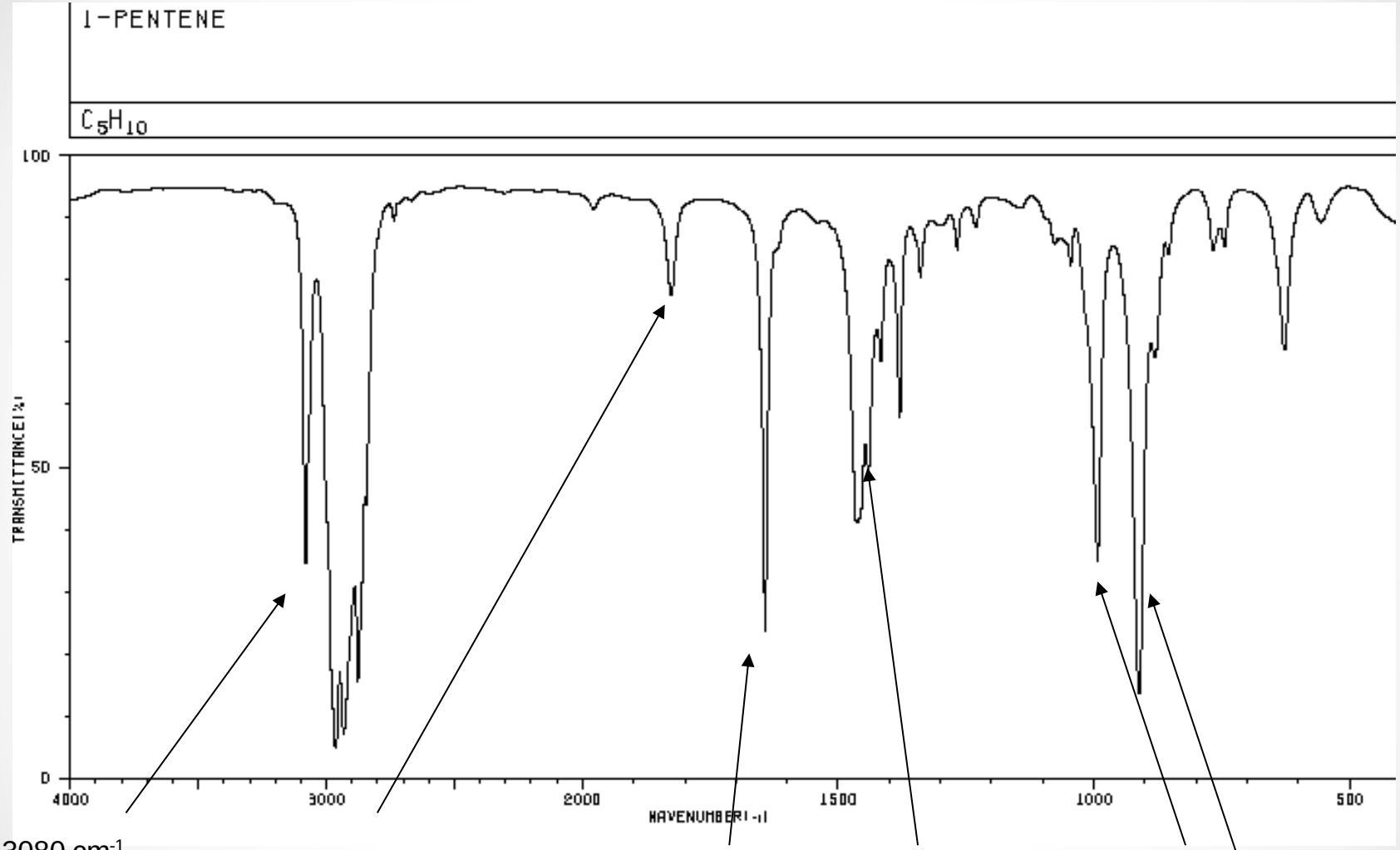


Simplified chart of several common functional groups with very characteristic absorptions.
s = strong, m = medium, w = weak, sh = sharp, br = broad.

Alkanes


HEXANE
C6H14
100
50
0
4000
3000
2000
1500
1000
500
WAVENUMBERS (cm-1)
2959 cm-1
νas (CH) CH3
2928 cm-1
νas (CH) CH2
2875 cm-1
νs (CH) CH3
2862 cm-1
νs (CH) CH2
1466 cm-1
δas (CH) CH3
1466 cm-1
δs (CH) CH2
1379 cm-1
δs (CH) CH3
726 cm-1
ρ (CH2)

Alkenes



3080 cm^{-1}
ν (CH) $C=CH_2$

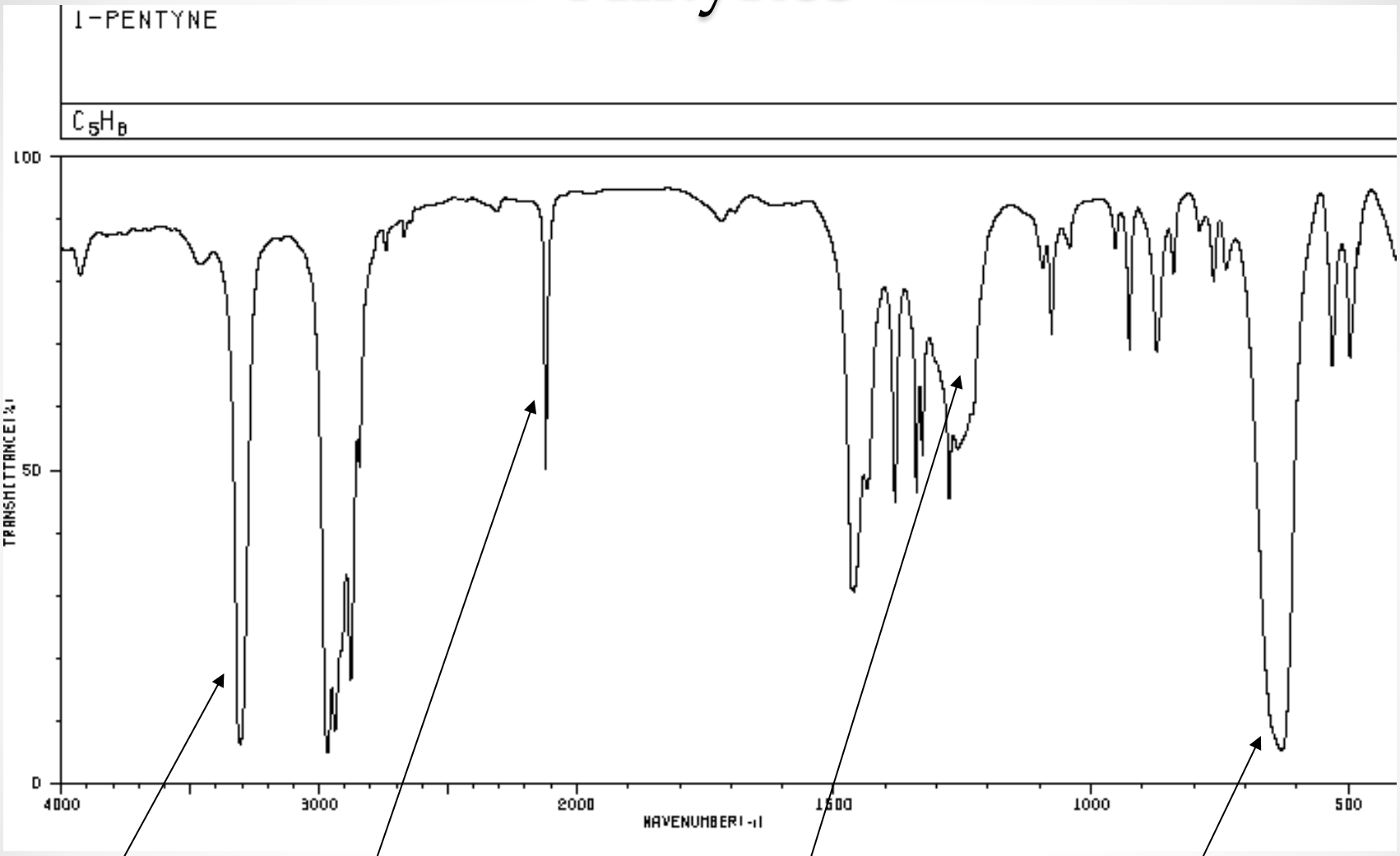
1826 cm^{-1}
$2*\gamma$ (CH) $C=CH_2$
overtone

1643 cm^{-1}
ν (C=C)

1417 cm^{-1}
δ_s (CH) $C=CH_2$
scissoring

993 i 912 cm^{-1}
γ (CH) $C=CH_2$
bendinging out of-plane

Alkynes



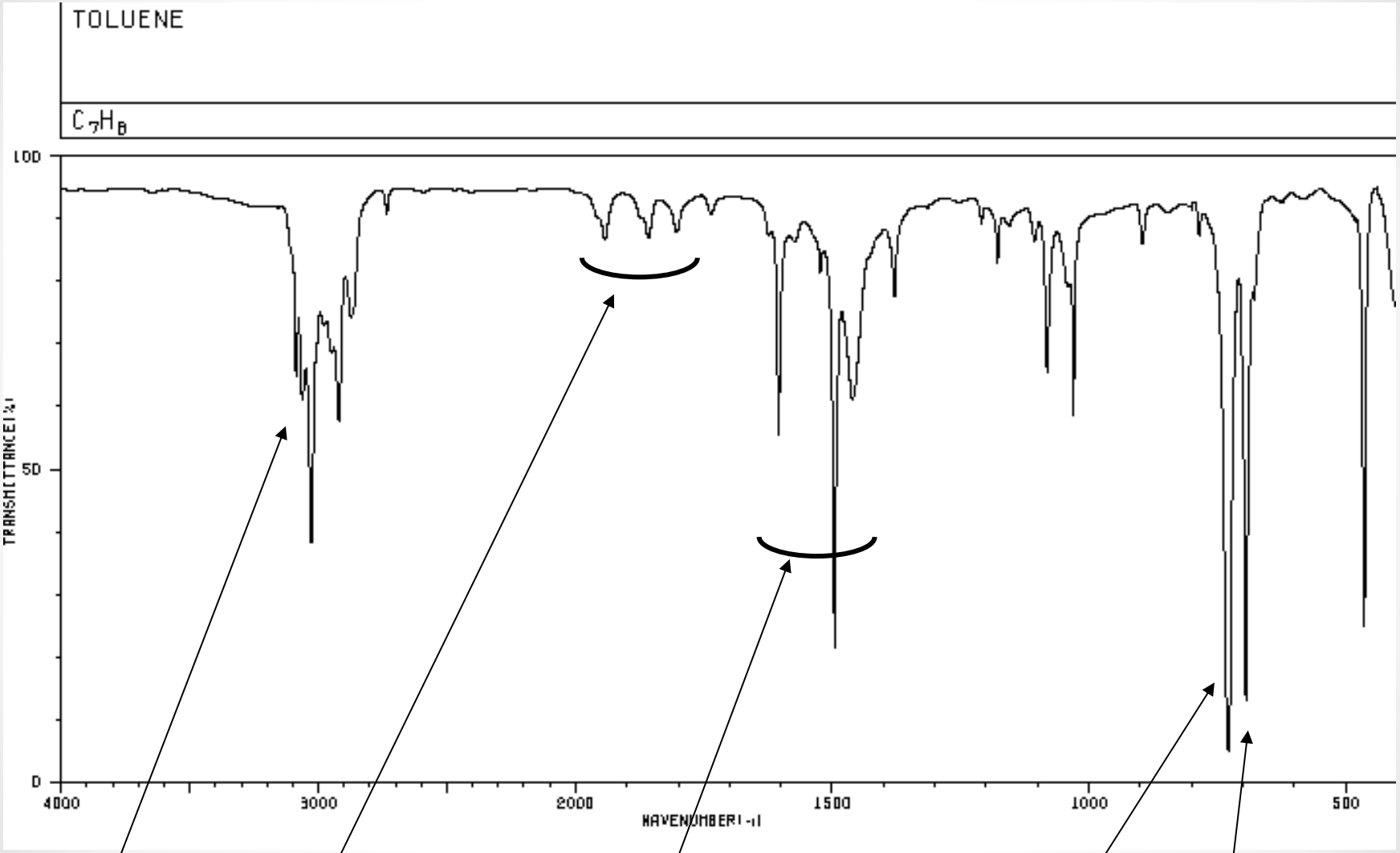
3307 cm^{-1}
n (CH) ≡—H

2120 cm^{-1}
ν (C≡C)

1259 cm^{-1}
2*γ (CH) ≡—H
overtone

630 cm^{-1}
γ (CH) ≡—H

Arenes



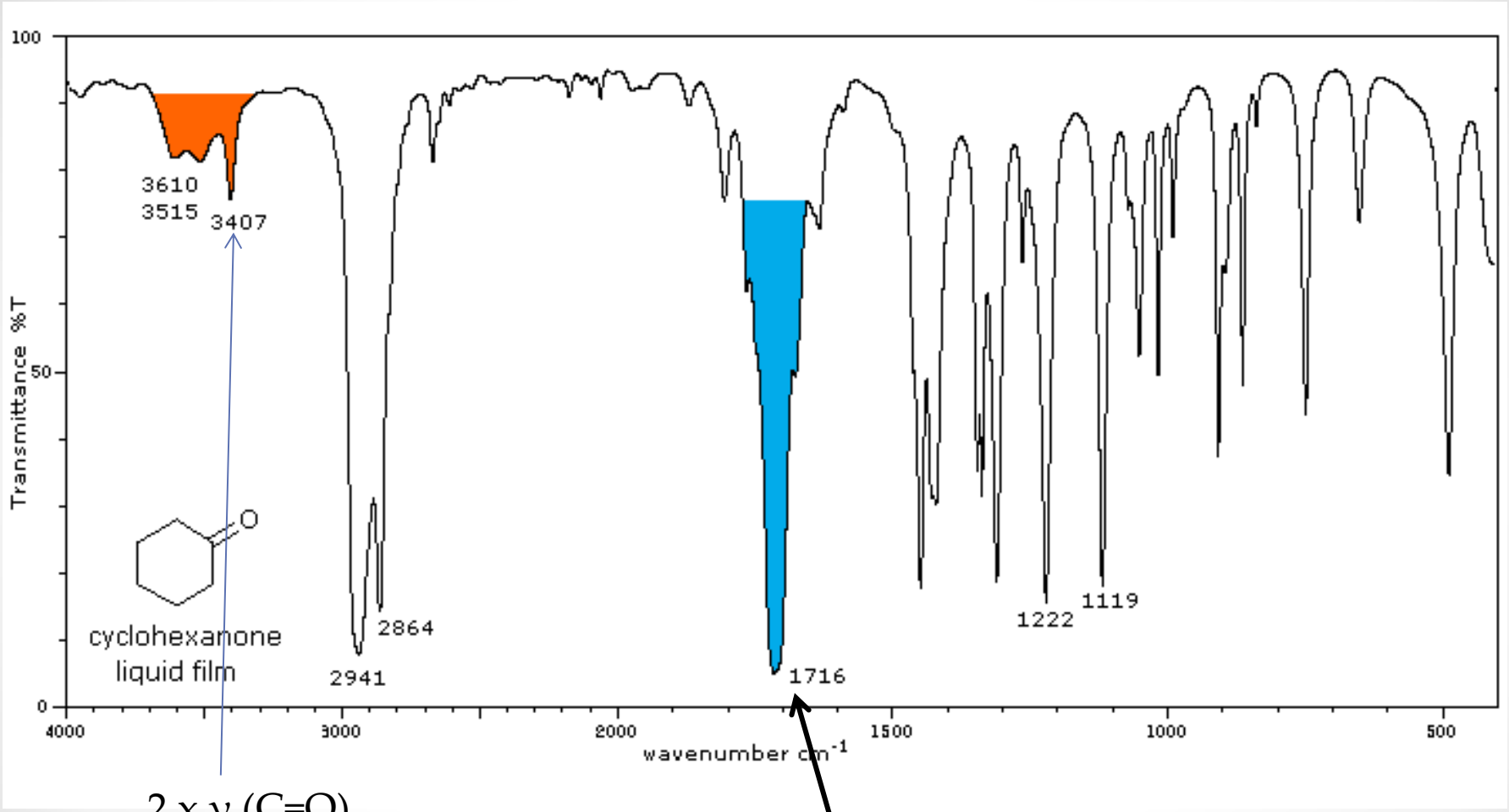
3028-3087 cm^{-1}
ν (CH) aromatic

2100-1700 cm^{-1}
overtones

1600, 1496, 1461 cm^{-1}
ν (C=C) aromatic

729 i 696 cm^{-1}
γ (CH) arom.
bending out of plane

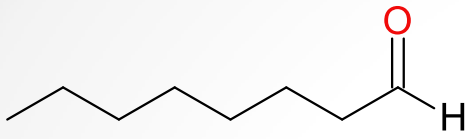
Carbonyl compounds - ketones



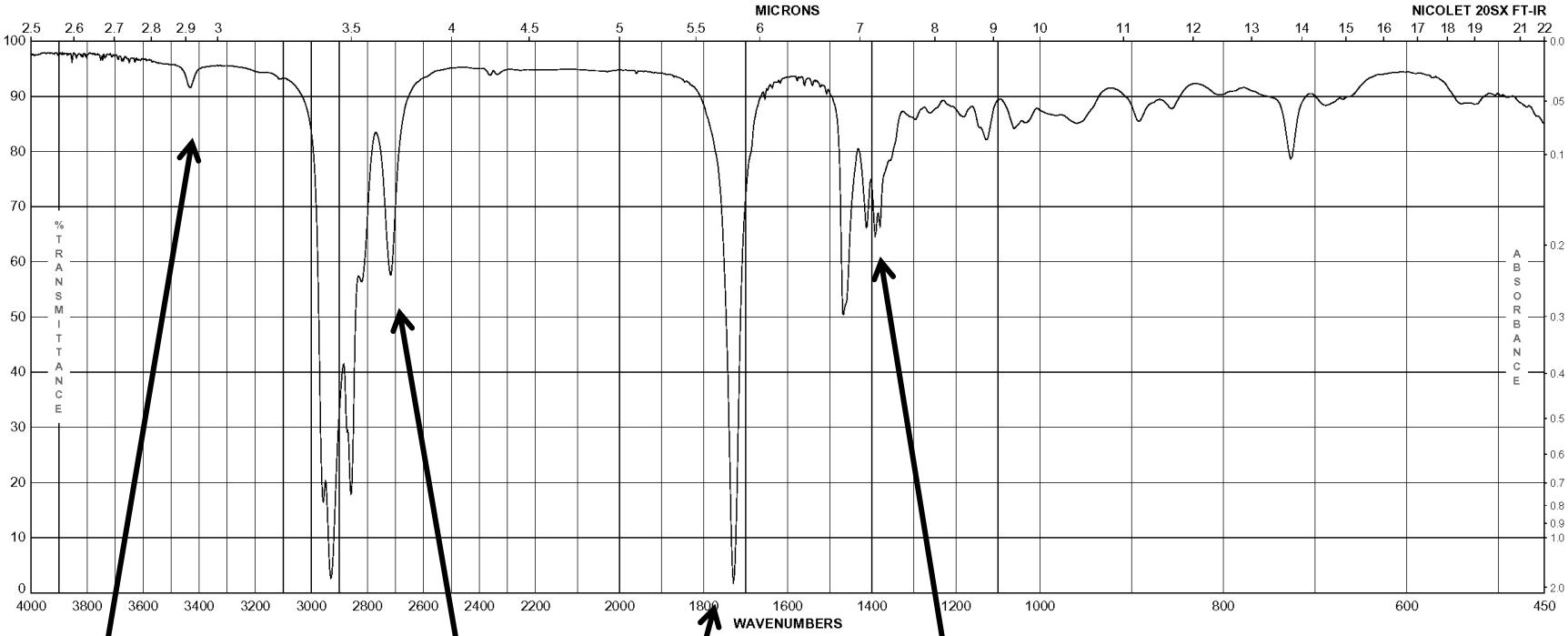
2 x ν (C=O) overtone

ν (C=O)

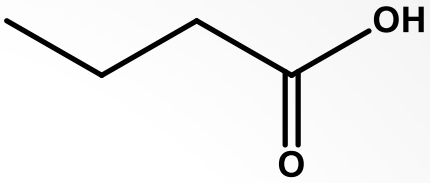
Carbonyl compounds - aldehydes

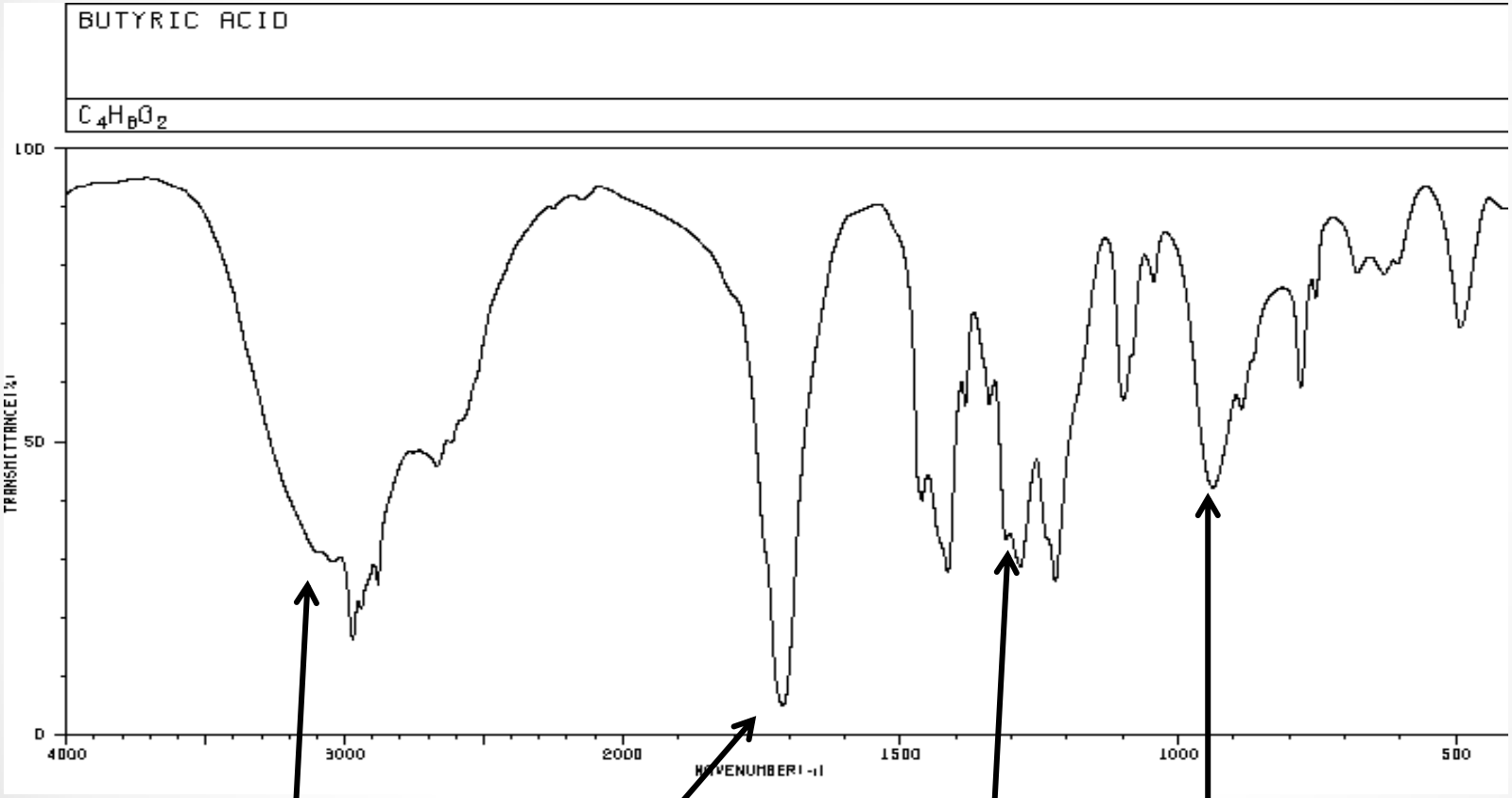


octanal

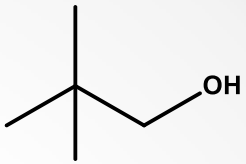


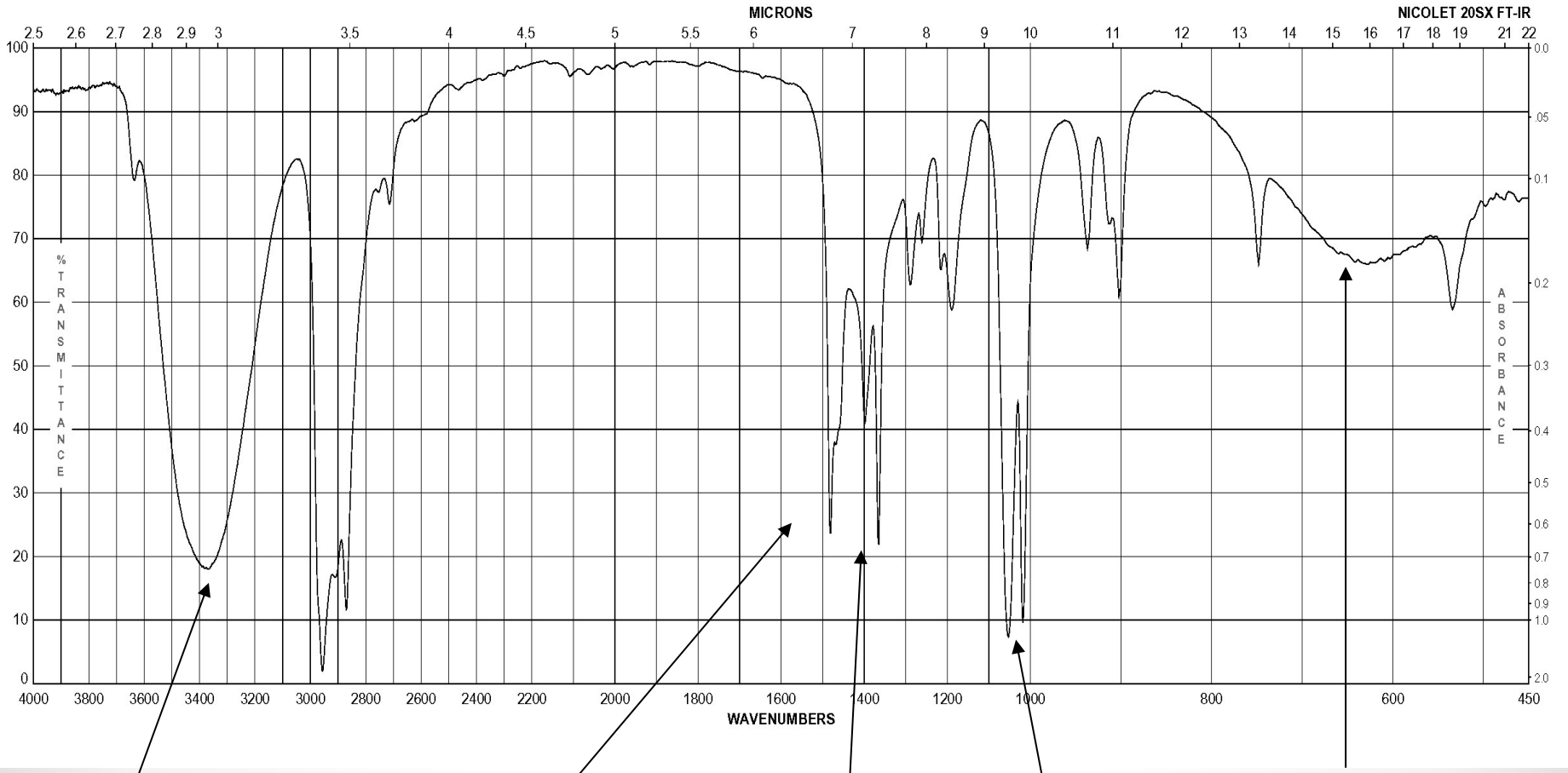
Carboxylic acids





2,2-dimethylpropan-1-ol





3350 cm^{-1}
ν (OH)

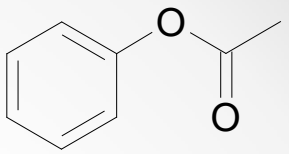
1480 cm^{-1}
δ_{as} CH_3 and δ_s CH_2

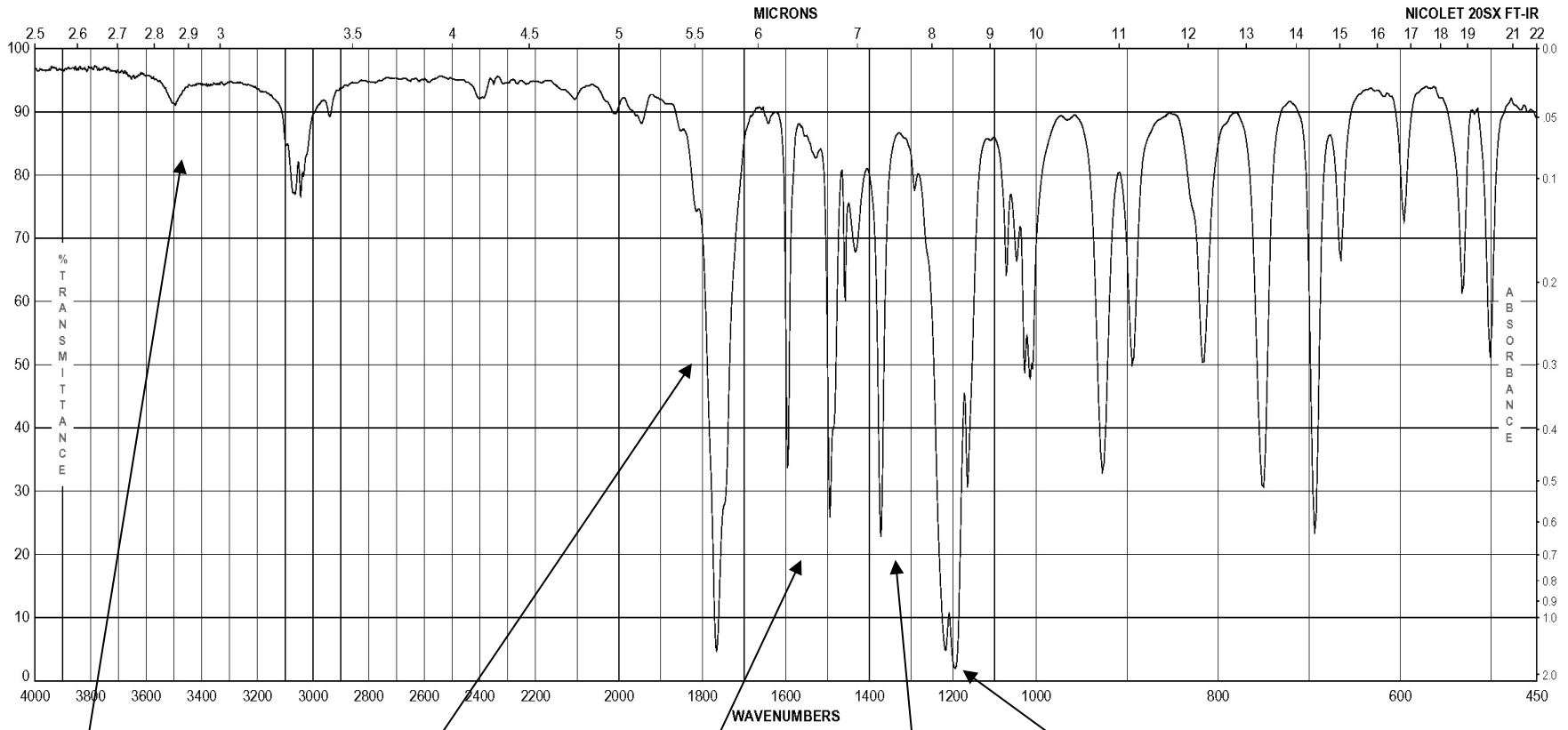
1390 and 1370 cm^{-1}
d_s CH_3

1000 i 1060 cm^{-1}
ν (C-O)

600 -650 cm^{-1}
γ (O–H)
bending out of plane

Phenyl acetate





overtone

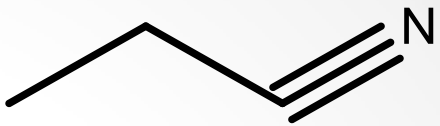
1770 cm^{-1}
ν (C=O)

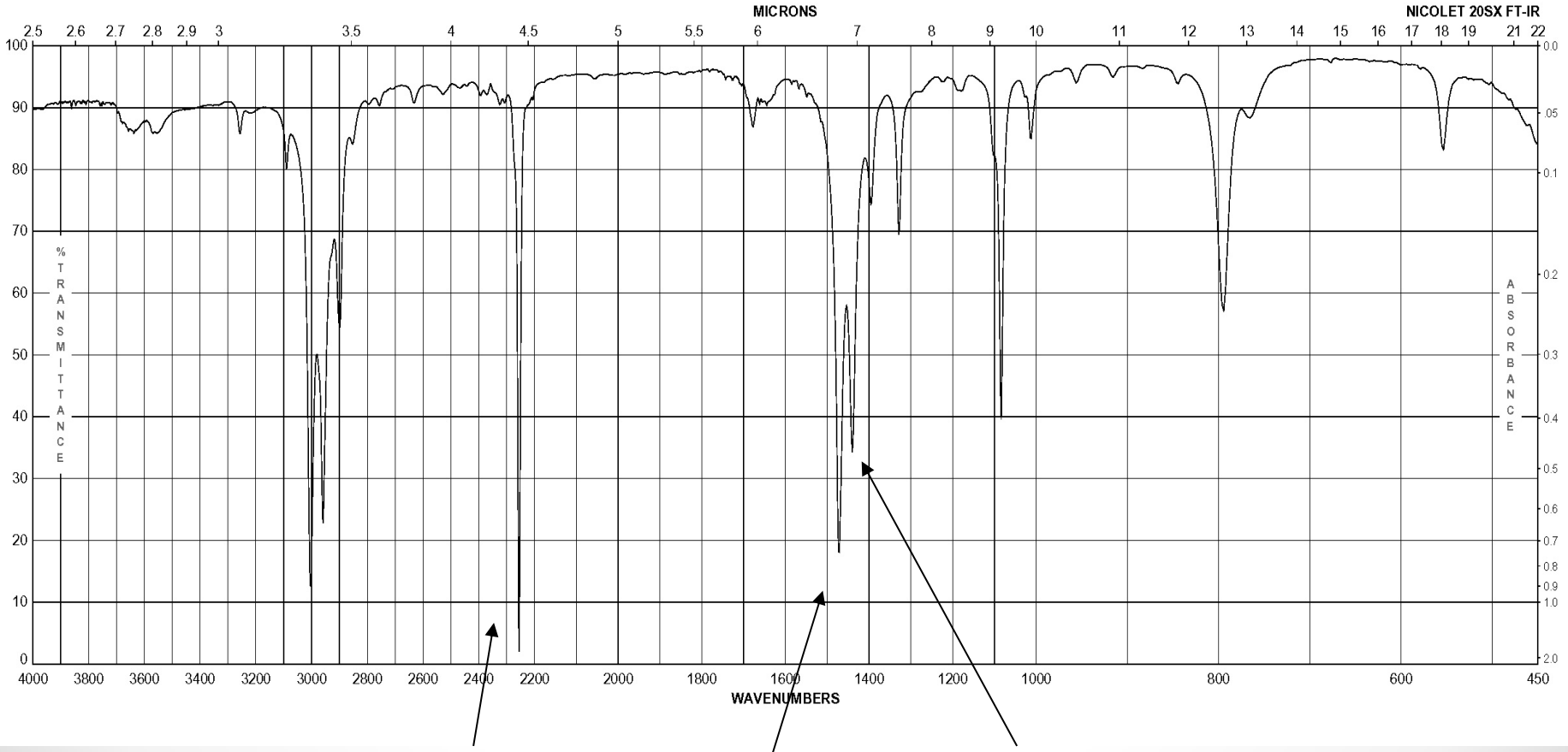
1600, 1493 cm^{-1}
ν (C=C)

1380 cm^{-1}
δ_s (C-H) CH_3

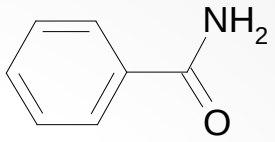
1195, 1210 cm^{-1}
ν (C-O)

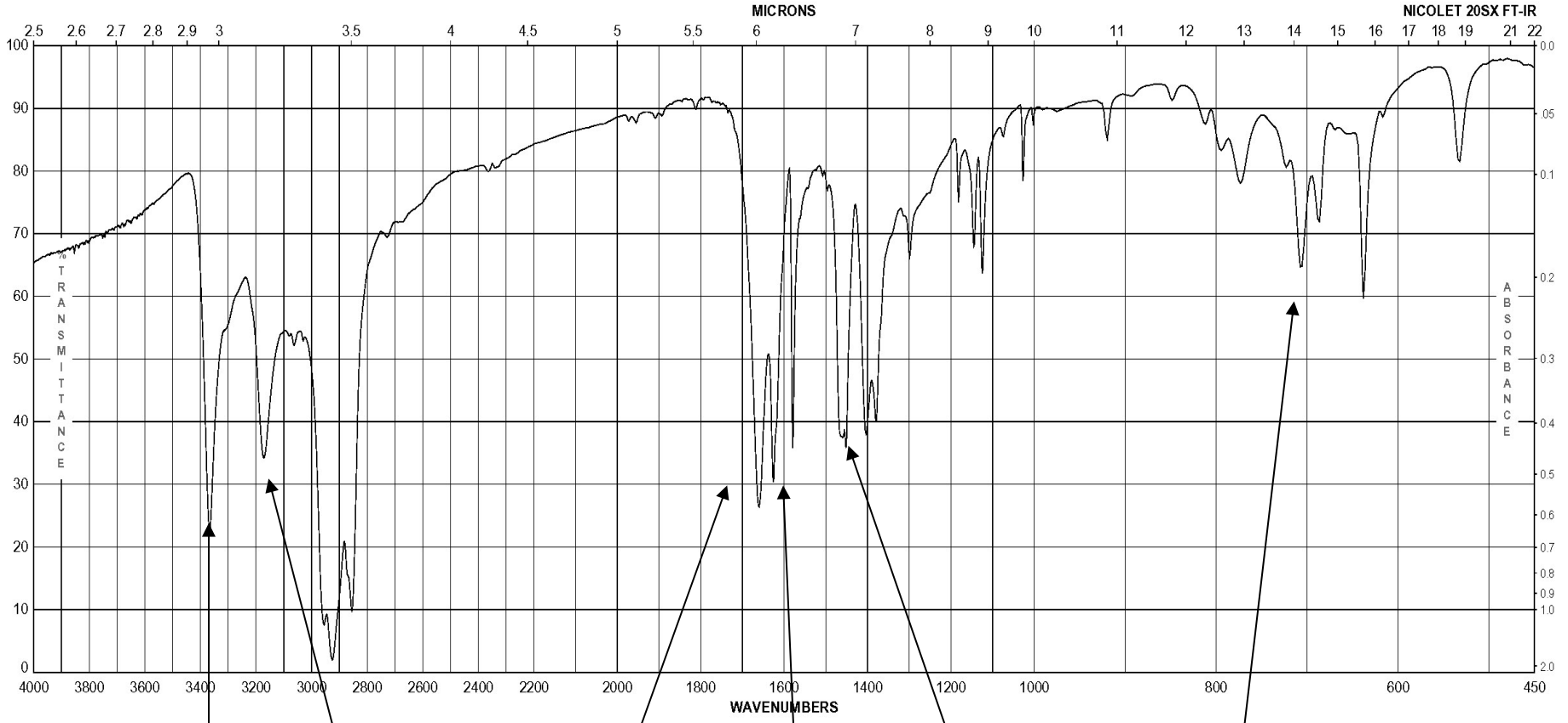
Propiononitrile





Benzamide





3380 cm^{-1}
ν_{as}(NH)

3180 cm^{-1}
ν_{s}(NH)

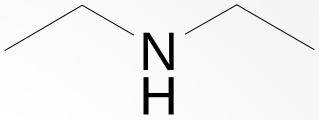
1660 cm^{-1}
ν (C=O)

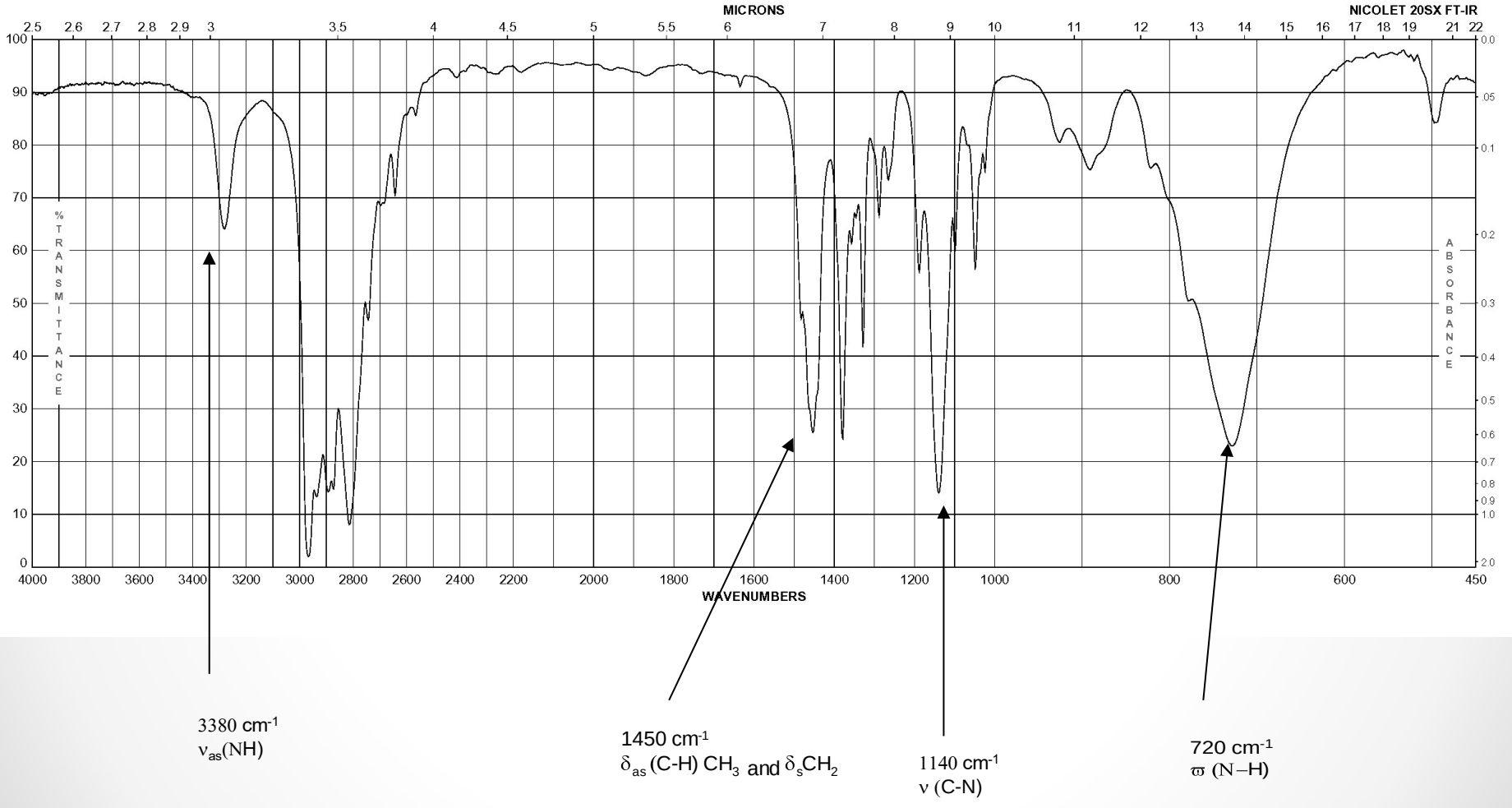
1620 cm^{-1}
δ (NH)

1400 cm^{-1}
ν (C-N)

710 cm^{-1}
ϖ (N–H)
bending out of plane

Diethylamine





3380 cm^{-1}
$\nu_{as}(NH)$

1450 cm^{-1}
δ_{as} (C-H) CH_3 and $\delta_s CH_2$

1140 cm^{-1}
ν (C-N)

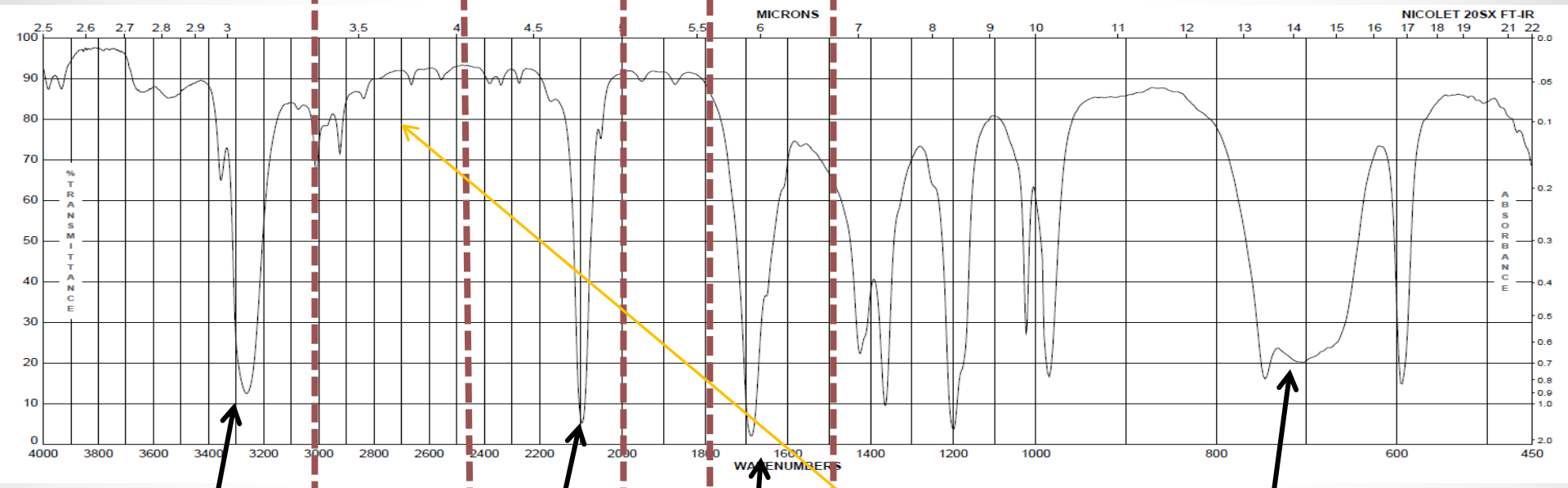
720 cm^{-1}
ϖ (N–H)

Ranges of absorption - summary

- 4000-3300 cm^{-1} N-H, O-H (stretching)
- 3100-3000 $_{sp2}$C-H (aryl, vinyl)
- 2500-2000 cm^{-1} C≡C and C≡N (stretching)
- 2000-1700 cm^{-1} C=O (stretching)
- 1500-1680 cm^{-1} C=C (stretching)
- Below 1500 cm^{-1} "fingerprint" region

Unknown compound – spectrum analysis

C_4H_4O DU = 3

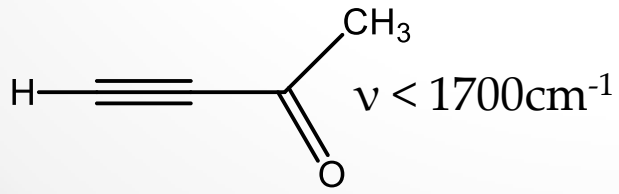


ν CNO? - H

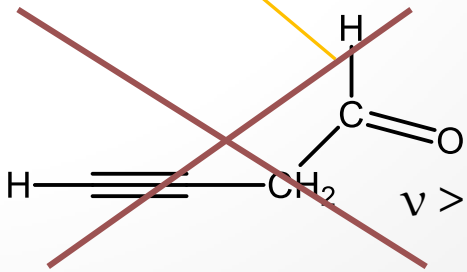
ν C≡C

ν C=O

γCNO? - H



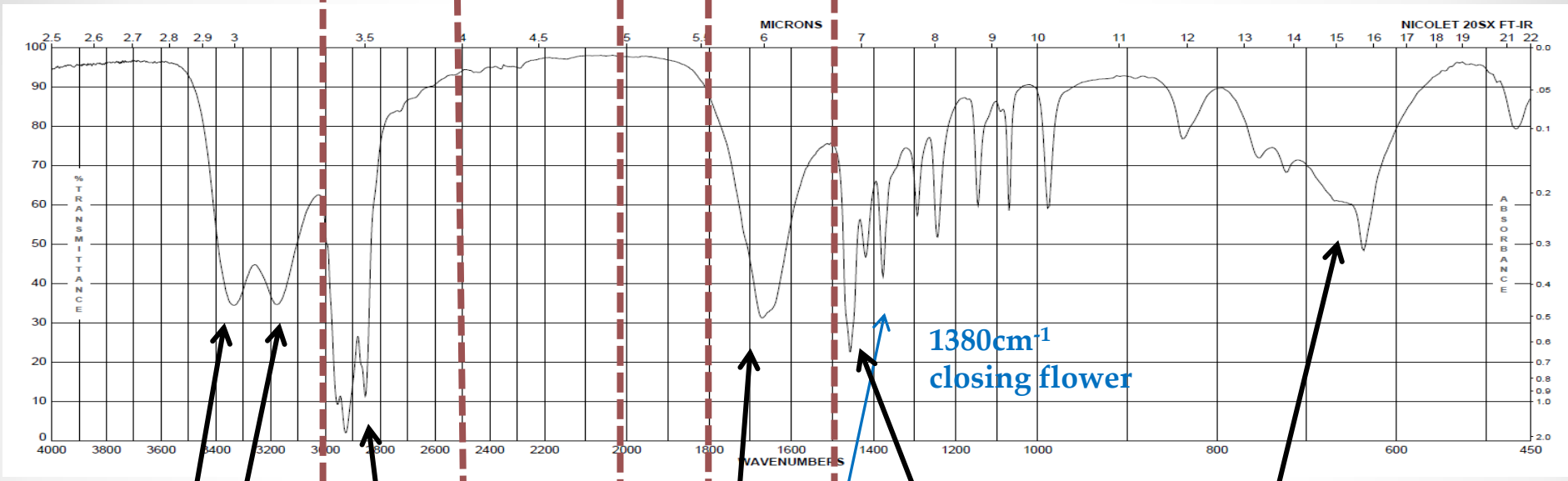
ν < 1700cm^{-1}



ν > 1700cm^{-1}

Unknown compound II – spectrum analysis

C_3H_6ClNO DU = 1



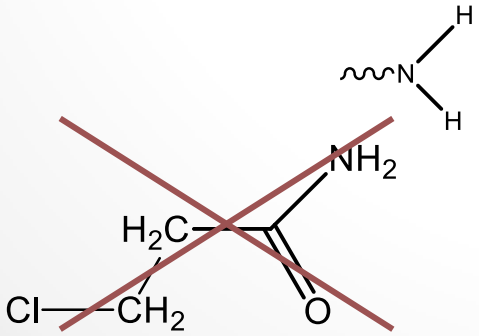
ν N–H
O-H ?
Amine
Amide
Alkohol?

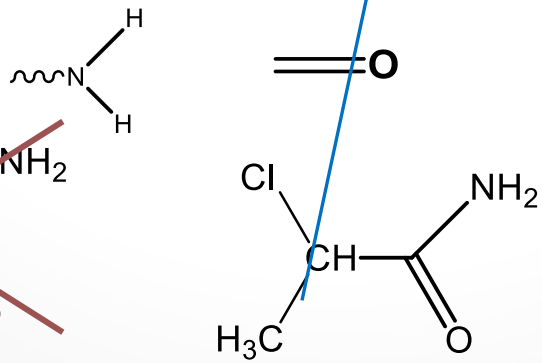
ν C-H alif.

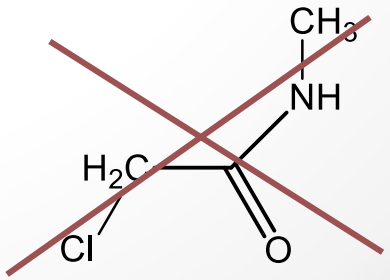
ν C=O

ν C-N

ω N – H
O-H ?

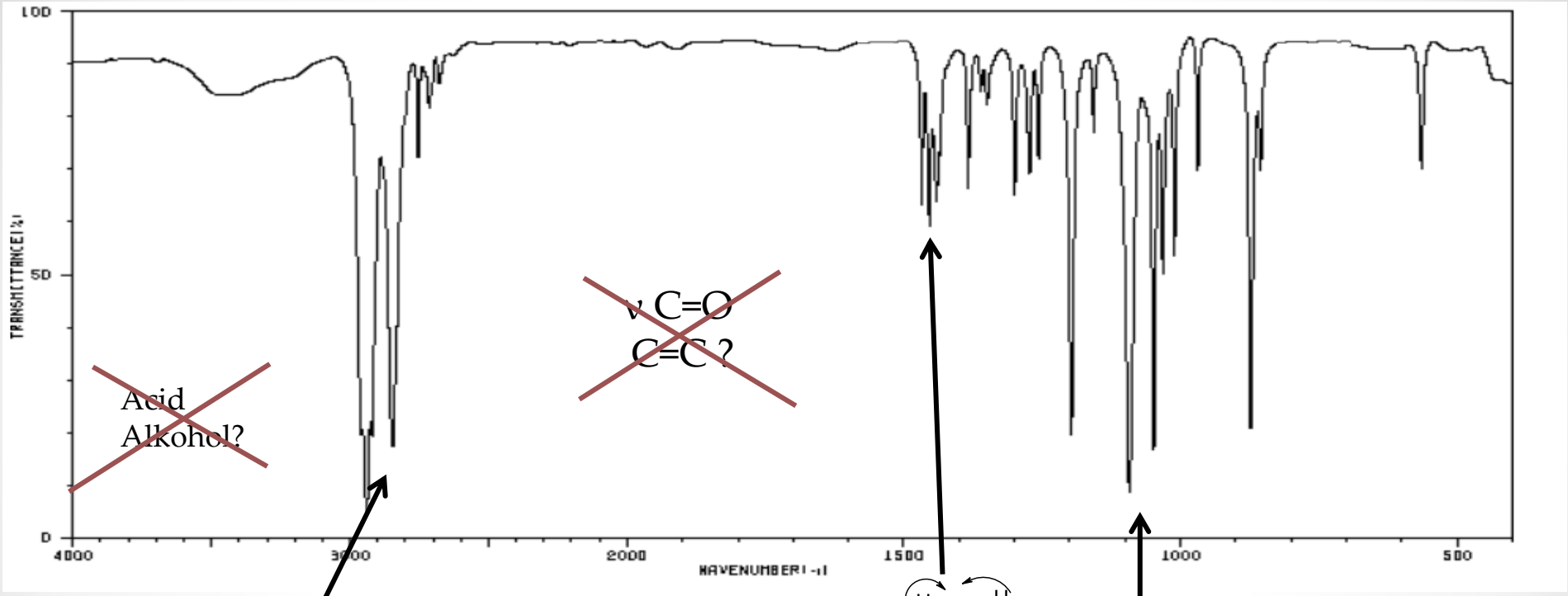






Unknown compound III – spectrum analysis

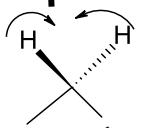
$C_5H_{10}O$ DU = 1



~~Acid~~
~~Alkohol?~~

~~ν C=O~~
~~C=C ?~~

ν C-H alif.



1466 cm^{-1}
δ_s (CH) CH_2

1100 cm^{-1}
ν (C-O)