

**ESPECTROMETRIA NA
REGIÃO DO
INFRAVERMELHO**
Outras absorções

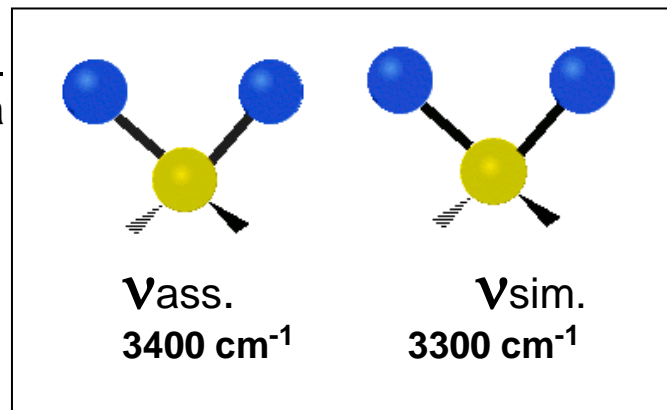
Profa. Veni Maria Andres Felli
guiluve@usp.br

ABSORÇÕES DE AMINAS

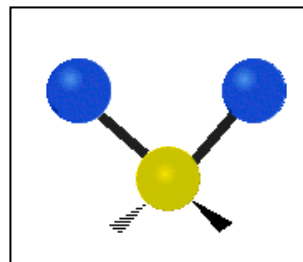
RNH_2 , RNHR'

νNH_2 aminas 1árias: 3500 a 3300 cm^{-1} – 2 bandas,
(muito característica, mas fraca em intensidade)

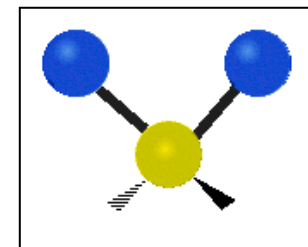
$\nu \text{N-H}$ aminas 2árias: 3310-3350 cm^{-1}
(1 banda fraca)



$\delta \text{N-H}$ no plano de aminas 1árias:
1640-1560 cm^{-1} (média a forte)
com overtone $\sim 3200 \text{ cm}^{-1}$

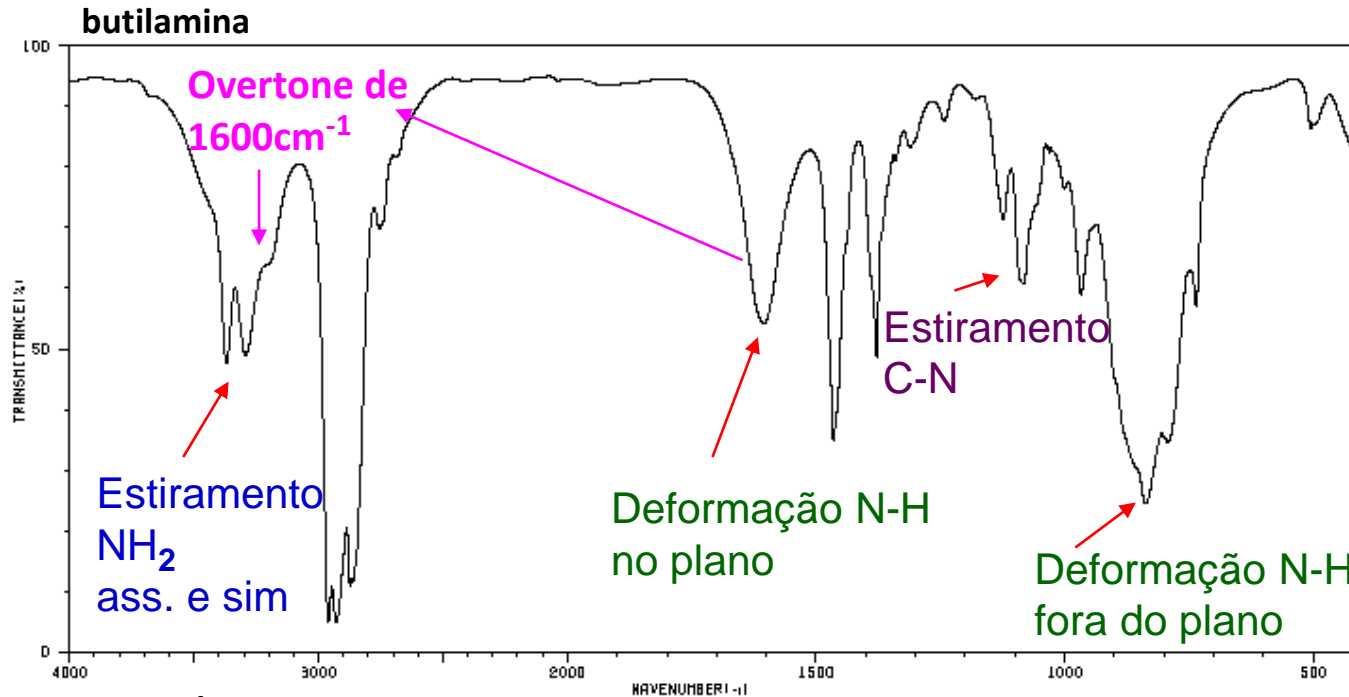


$\delta \text{N-H}$ em onda de aminas 1árias e 2árias:
 $\sim 800 \text{ cm}^{-1}$ (média a forte, usualmente larga)



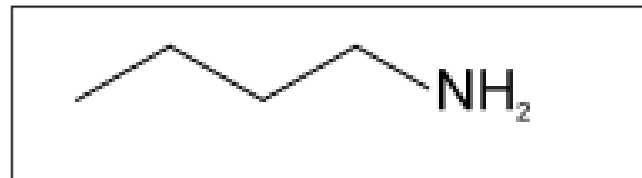
$\nu \text{C-N}$ 1350 a 1000 cm^{-1}

ABSORÇÕES DE AMINAS



ABSORBÂNCIA

3369	46	1606	62	1083	58	498	84
3293	47	1465	33	1001	74		
2960	4	1379	46	867	57		
2928	4	1340	77	837	23		
2874	10	1312	79	792	33		
2862	10	1243	84	736	55		
2767	66	1124	68	606	84		



ABSORÇÕES DE SAIS DE AMÔNIO



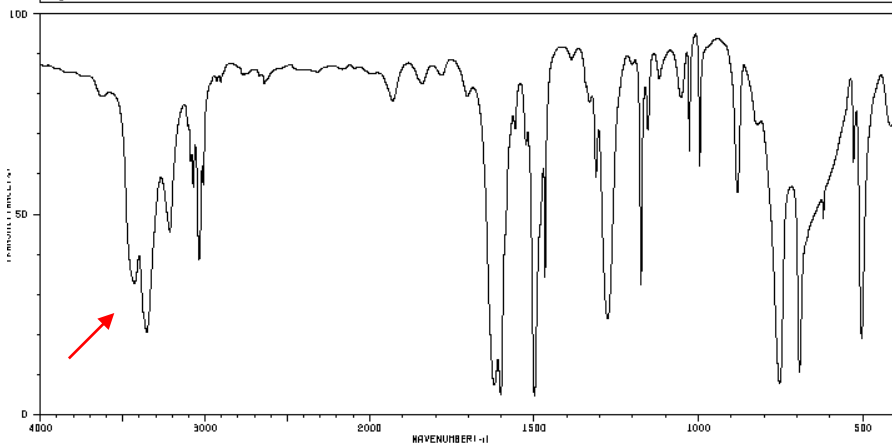
ν N-H 3300-2600 cm^{-1}
(banda larga $\sim 2100 \text{ cm}^{-1}$)

δ N-H 1610-1500 cm^{-1}

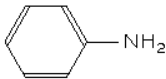
- Sal 1ário- ass. 1610 cm^{-1}
sim 1500 cm^{-1}
- Sal 2ário – 1610-1550 cm^{-1}
- Sal 3ário – absorção fraca

ABSORÇÕES DE SAIS DE AMÔNIO

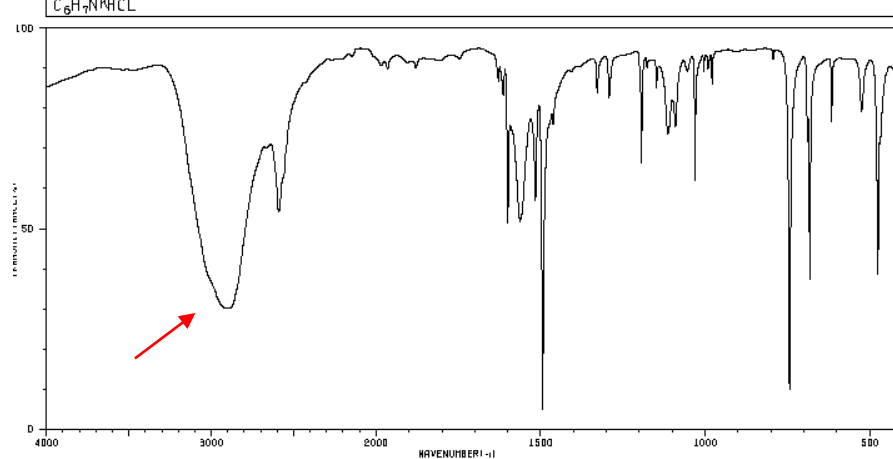
HIT-NO=1244	SCORE= ()	SDBS-NO=905	IR-NIDA-15056 : LIQUID FILM
ANILINE			
C_6H_7N			



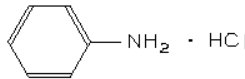
3623	77	3010	57	1706	77	1332	74	996	50
3429	32	2930	81	1621	7	1312	57	881	53
3354	20	2904	78	1601	5	1277	29	754	8
3214	44	2640	78	1567	70	1176	32	693	10
3088	82	2627	81	1525	66	1154	68	620	47
3072	55	1929	77	1498	4	1053	77	529	50
3037	38	1839	78	1467	34	1028	64	504	18

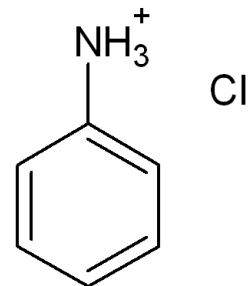


HIT-NO=1472	SCORE= ()	SDBS-NO=1452	IR-NIDA-04236 : KBR DISC
ANILINE HYDROCHLORIDE			
$C_6H_7NH_4Cl$			

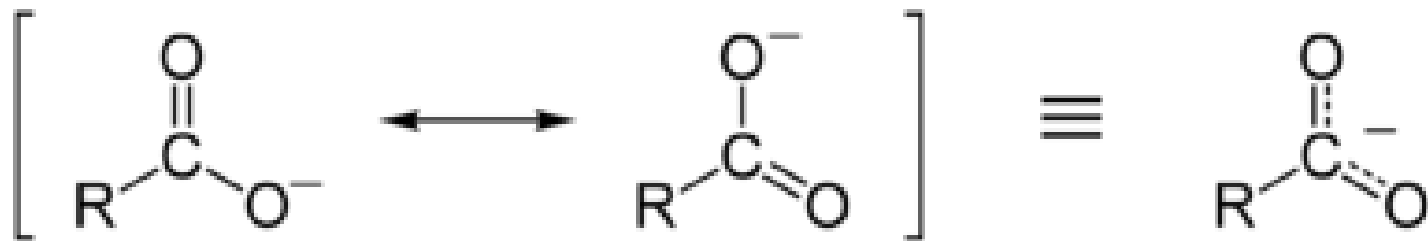


2912	26	1600	48	1194	64	992	86	476	37
2902	29	1562	50	1149	81	979	84	469	68
2590	52	1516	55	1114	70	744	8		
2562	60	1494	4	1090	72	690	68		
1965	86	1462	72	1054	86	683	36		
1828	84	1329	81	1031	80	616	74		
1614	79	1292	78	1006	86	526	77		





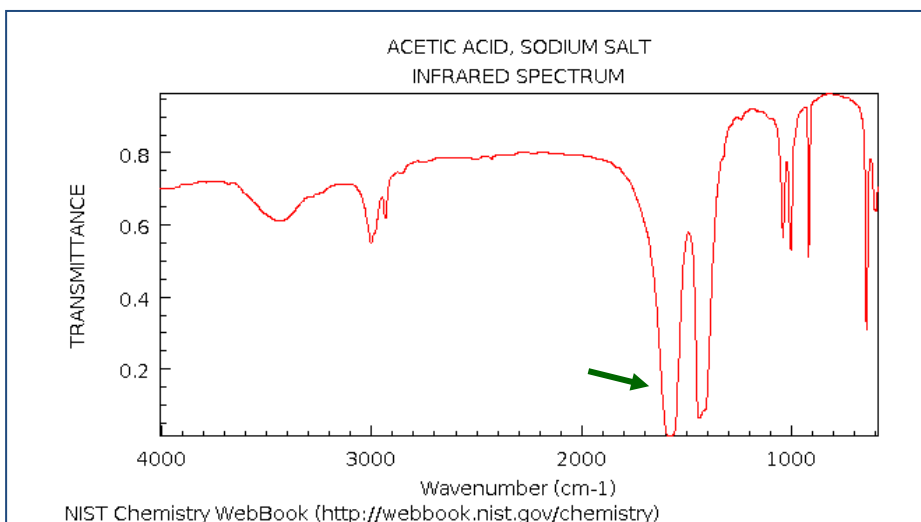
ABSORÇÕES DE CARBOXILATOS



Estiramento

- **assimétrico**
- **simétrico**

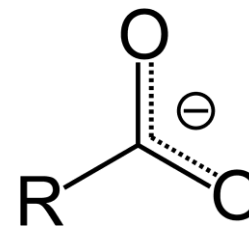
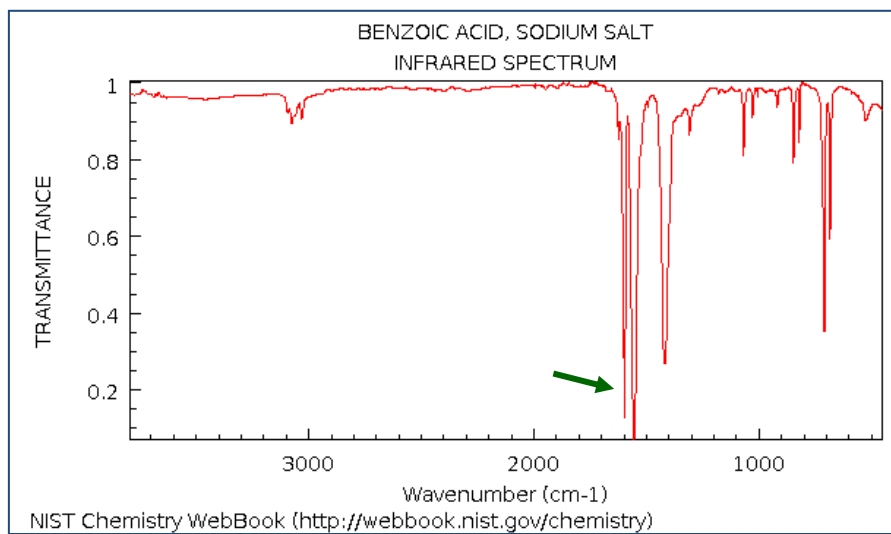
ABSORÇÕES DE CARBOXILATOS



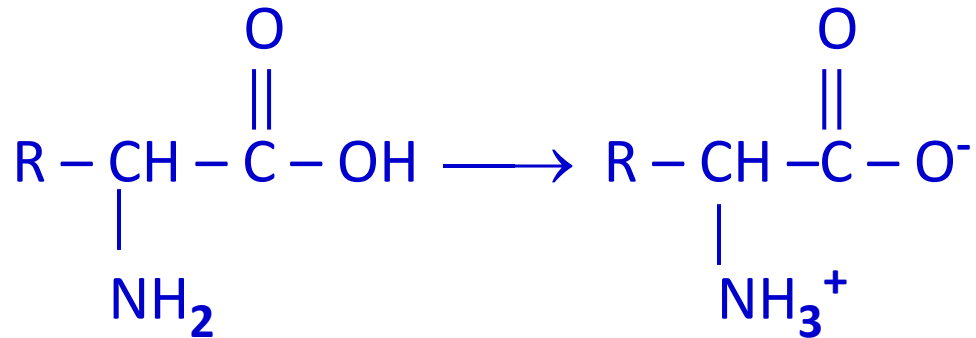
ν assim. COO^- $\sim 1600 \text{ cm}^{-1}$

ν sim. COO^- $\sim 1400 \text{ cm}^{-1}$

↓ Frequência de absorção devido à ressonância C=O com maior caráter de ligação simples



ABSORÇÕES DE AMINOÁCIDOS



ν N-H

ν C=O

ν O-H

δ N-H

(no plano e fora do plano)

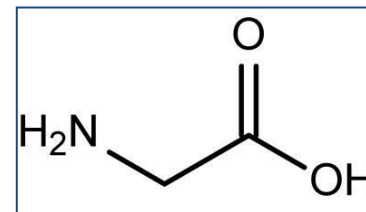
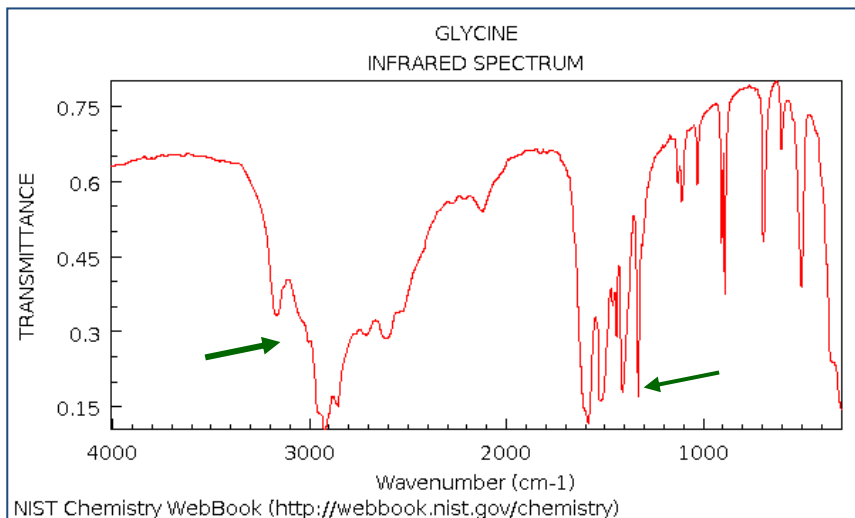
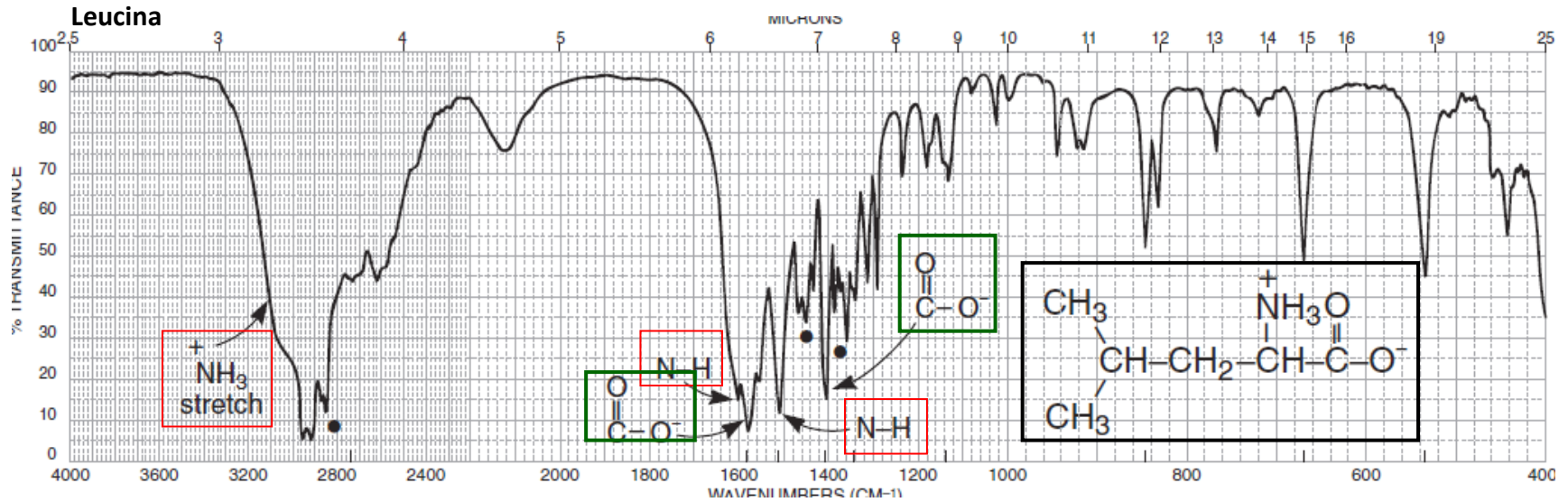
ν N-H⁺ (muito larga)

ν COO⁻ (ass. e sim.)

δ N-H (ass. e sim.)

**Compostos zwitteriônico
(sal interno)**

ABSORÇÕES DE AMINOÁCIDOS

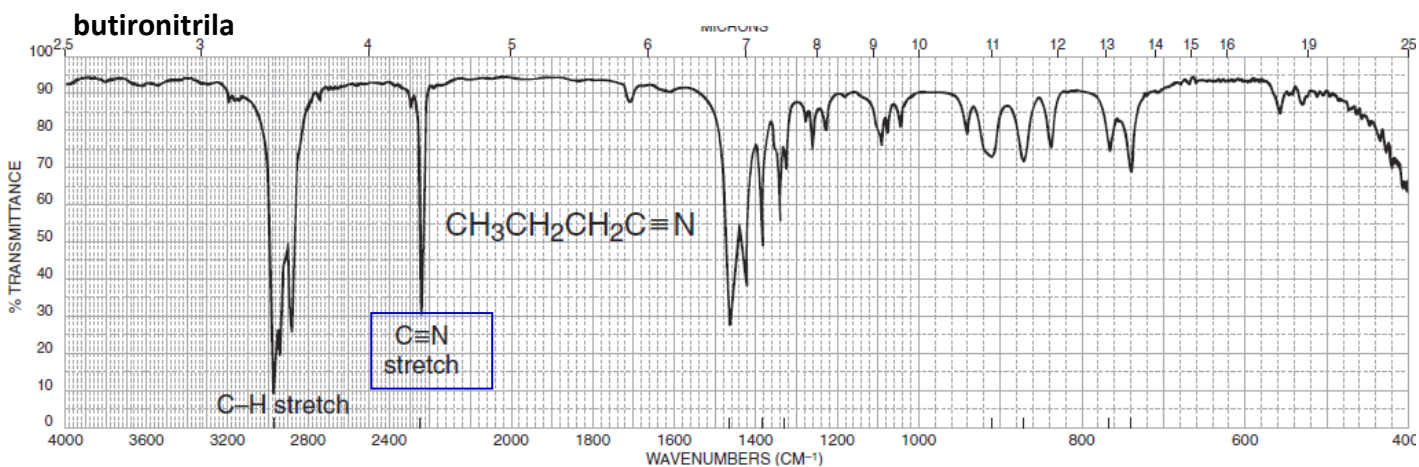


Base livre ou na forma zwitteriônica ?

ABSORÇÃO DE NITRILA

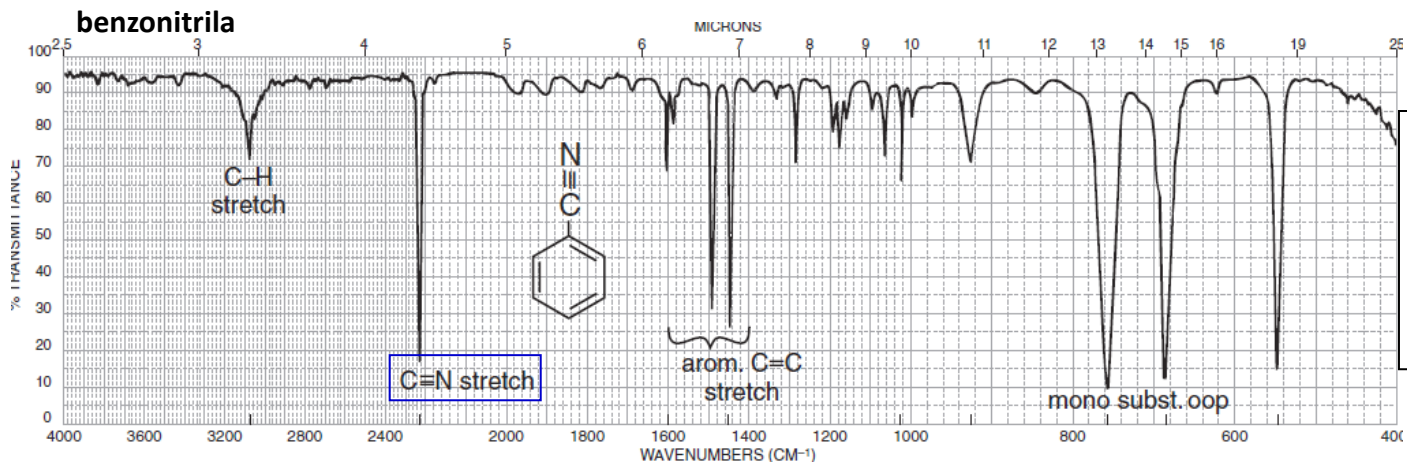
$R - C \equiv N$ C com hibridização sp

butironitrila



$\nu C \equiv N \sim 2250 \text{ cm}^{-1}$
absorção aguda e de
intensidade média

benzonitrila



Conjugação

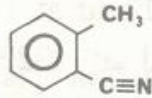
$\nu C \equiv N \sim 2230 \text{ cm}^{-1}$

↓ Frequência

↑ Intensidade

ABSORÇÃO DE NITRILA

11977-6 CAS [529-19-1]
o-Tolunitrile, 98%

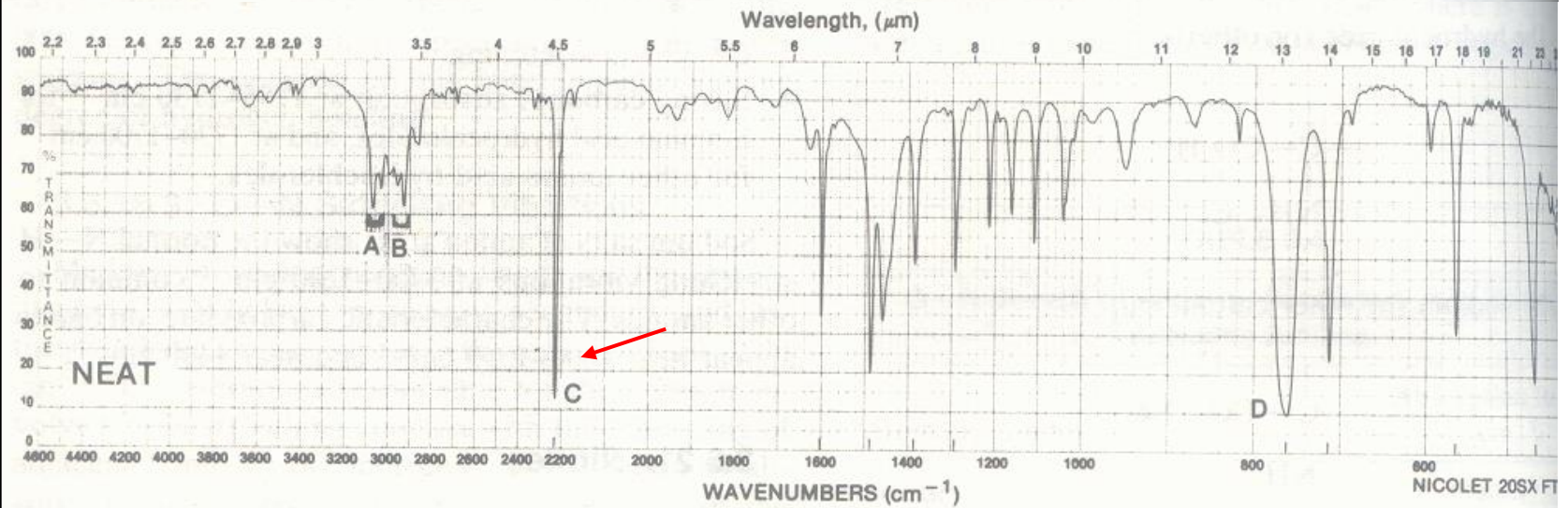


FW 117.15
mp 13°C
bp 205°C

d 0.989
Fp 184°F
n_D 1.5279

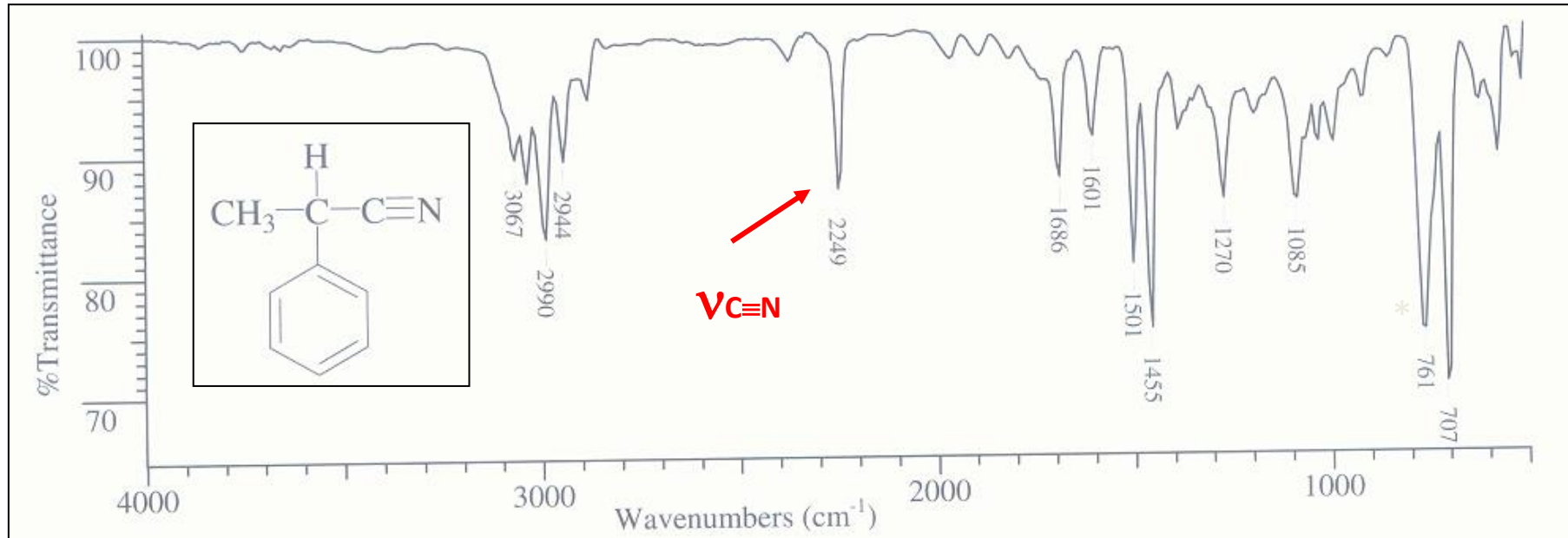
IR III, 1128D
Merck 10,9367

2225.6	1384.5	712.0
1601.6	1291.2	562.6
1486.9	760.9	458.9



ABSORÇÃO DE NITRILA

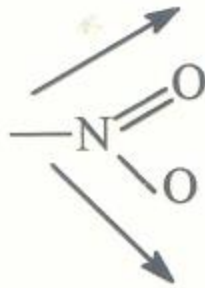
α -metilbenzilcianonitrila



ABSORÇÕES DE NITROCOMPOSTOS

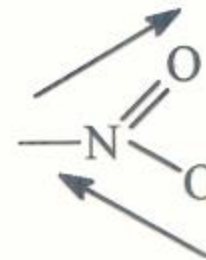
ESTIRAMENTO
SIMÉTRICO

NITRO



($\sim 1350 \text{ cm}^{-1}$)

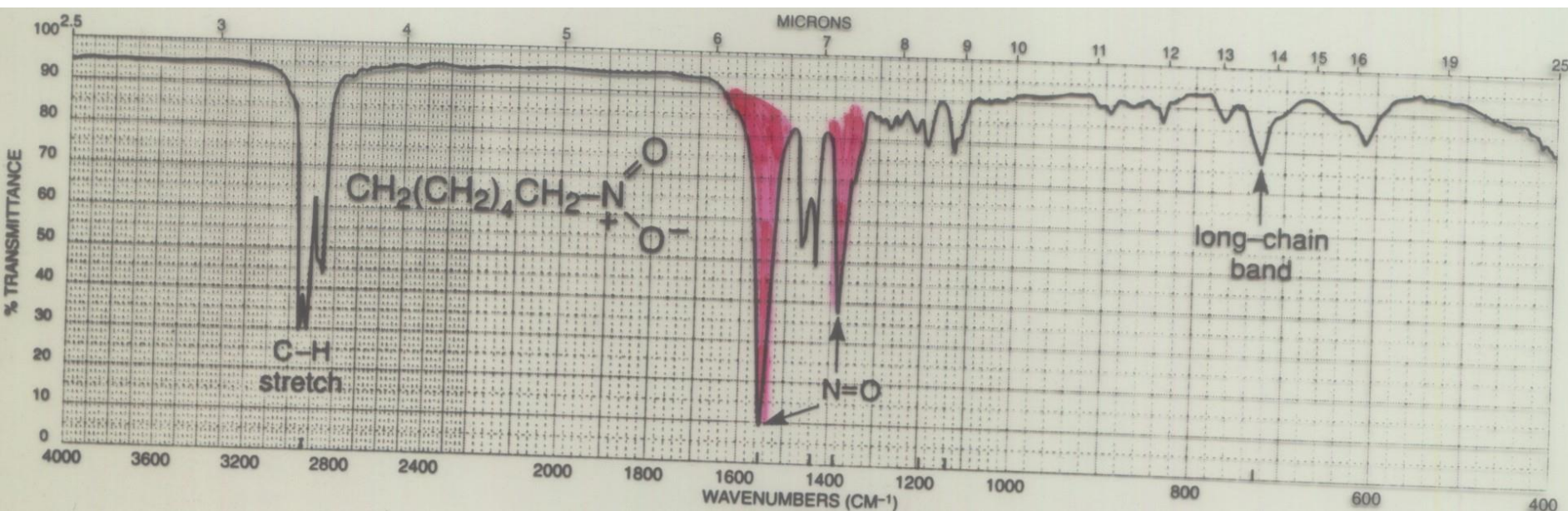
ESTIRAMENTO
ASSIMÉTRICO



($\sim 1550 \text{ cm}^{-1}$)

ABSORÇÕES DE NITROCOMPOSTOS

R-NO₂



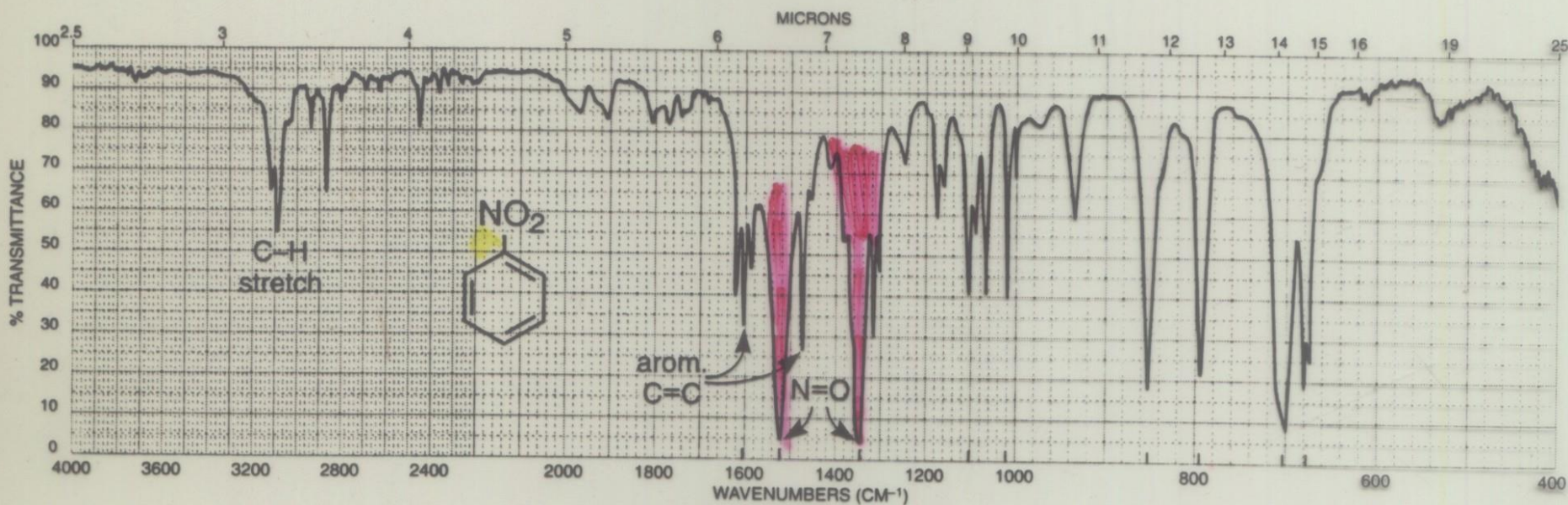
Alifáticos

Vass. NO₂ 1600-1530 cm⁻¹ (forte)

Vsim. NO₂ 1390-1300 cm⁻¹ (médio)

ABSORÇÕES DE NITROCOMPOSTOS

R-NO₂

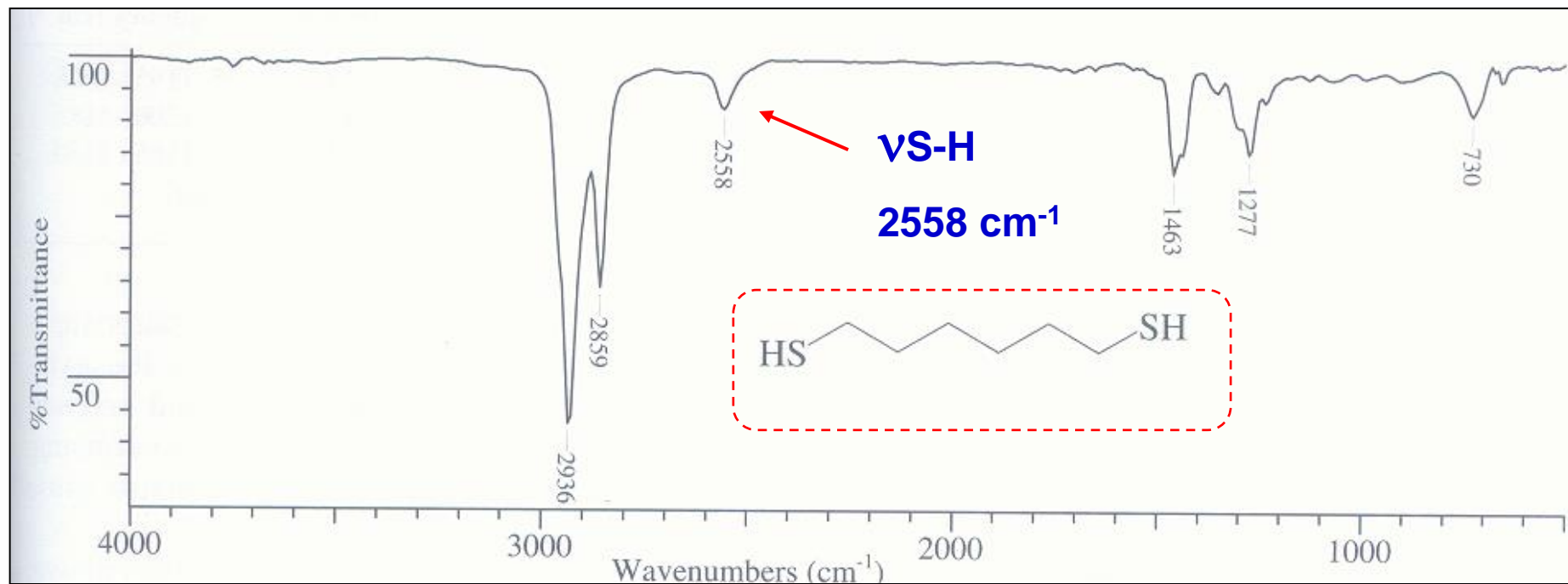


Aromáticos

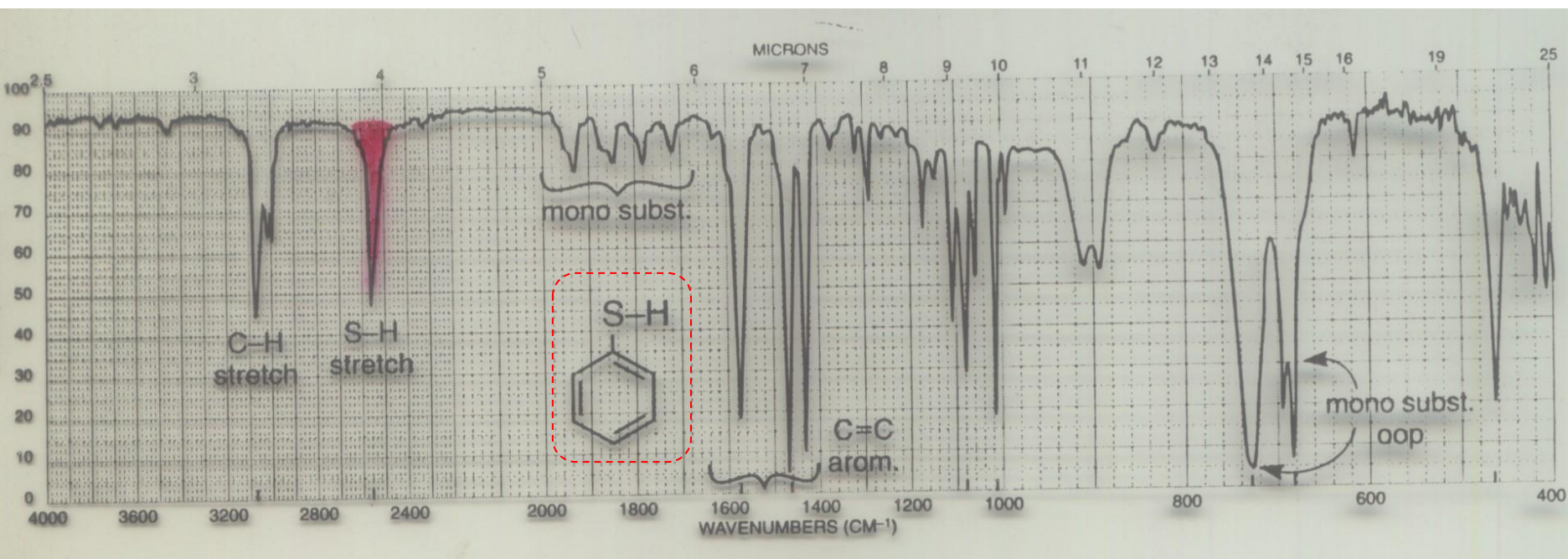
Vass. NO₂ 1550-1490 cm⁻¹ (forte)

Vsim. NO₂ 1355-1315 cm⁻¹ (forte)

ABSORÇÕES DE COMPOSTOS SULFURADOS

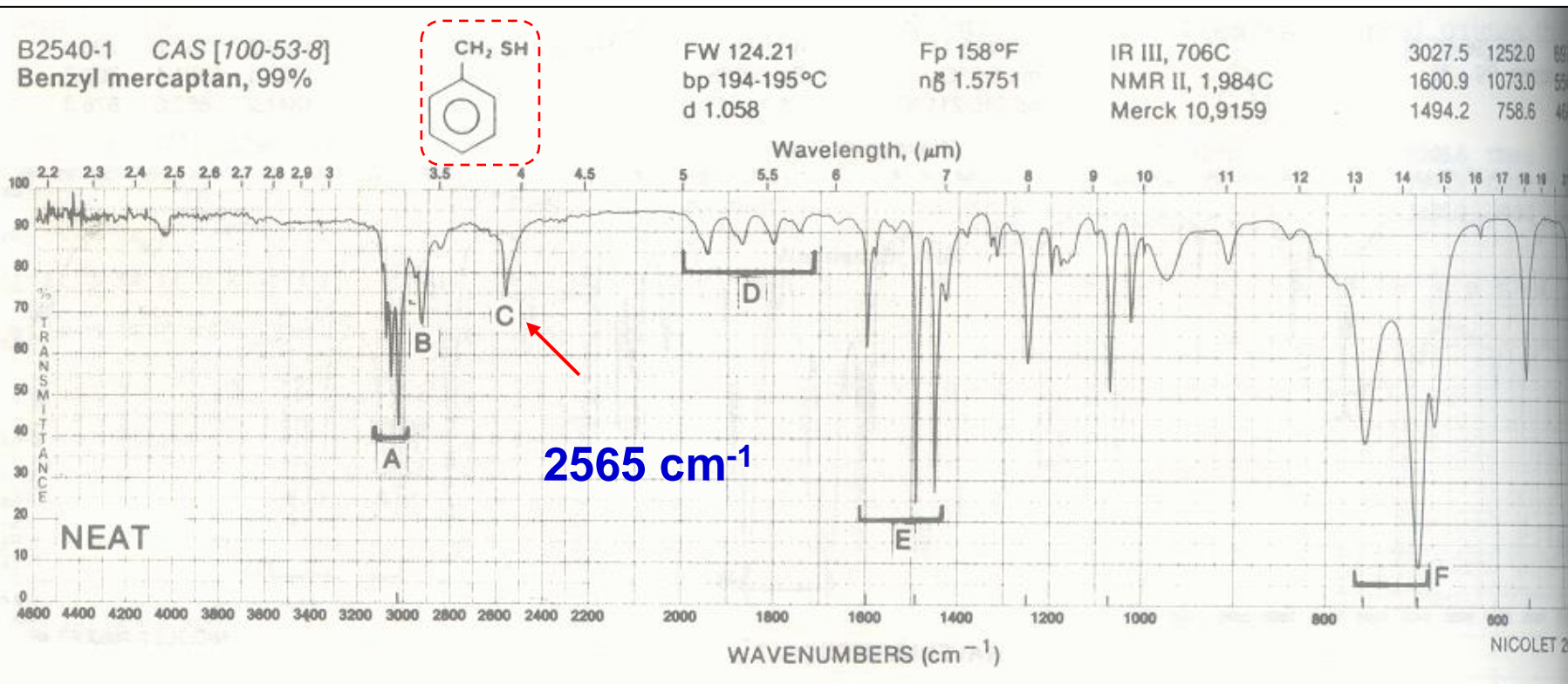


ABSORÇÕES DE COMPOSTOS SULFURADOS

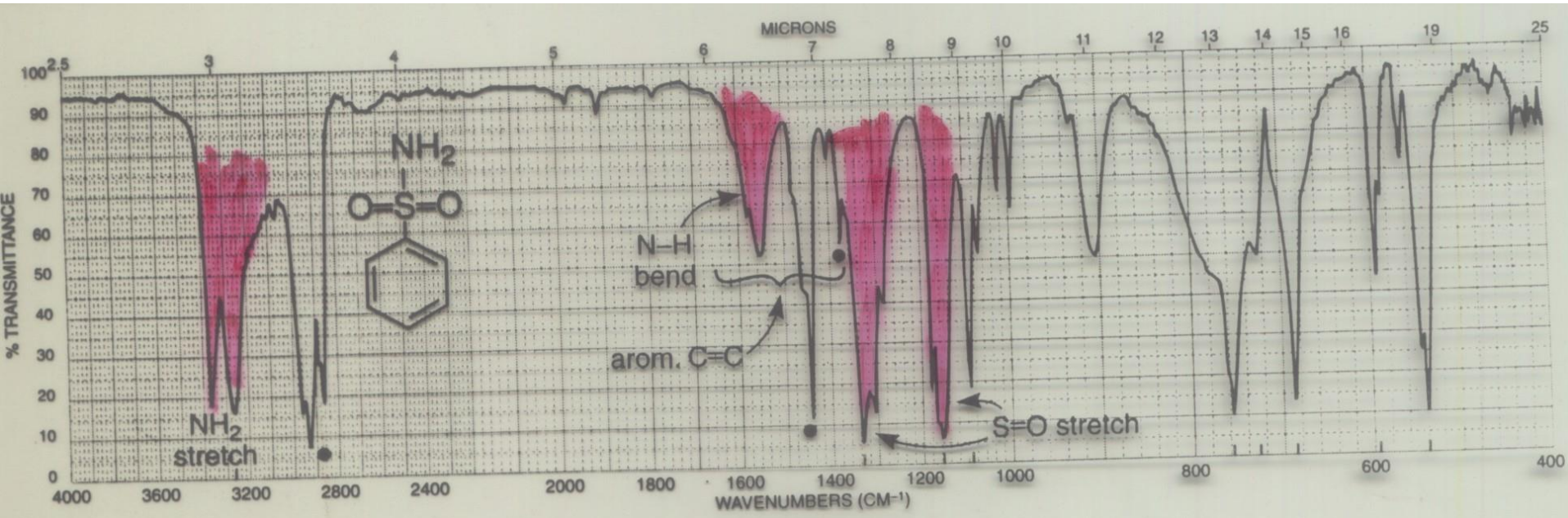


VS-H ~ 2550 cm^{-1}

ABSORÇÕES DE COMPOSTOS SULFURADOS



ABSORÇÕES DE COMPOSTOS SULFURADOS



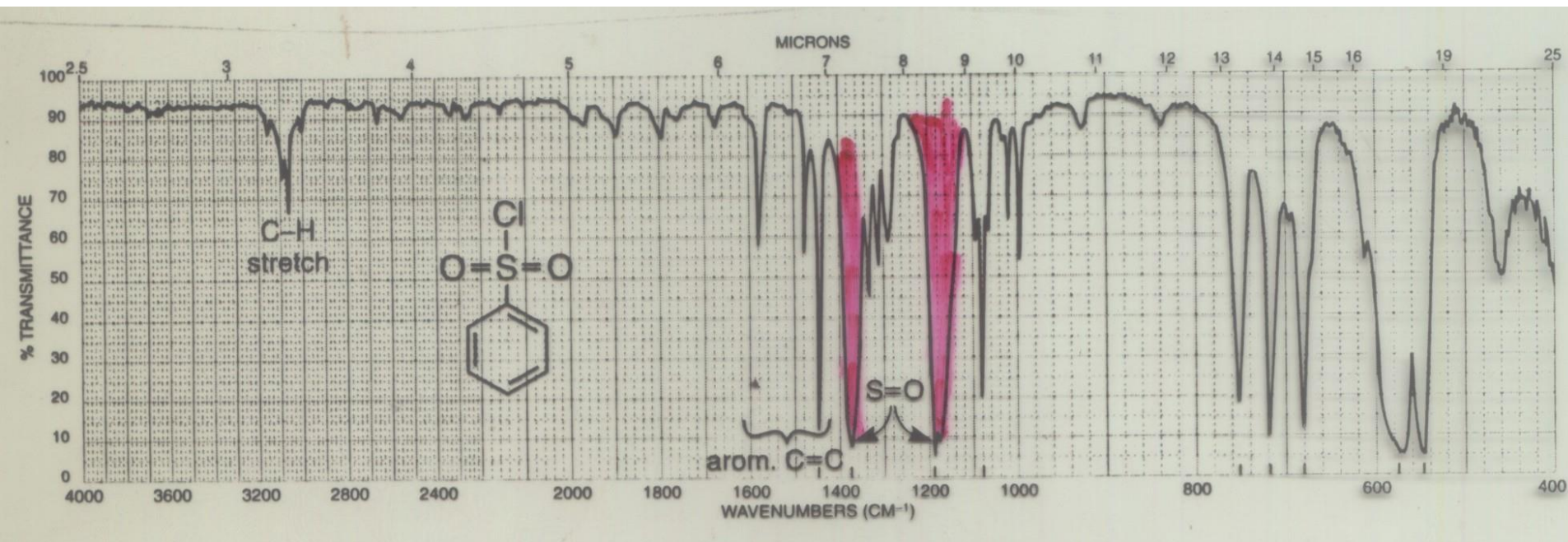
Sulfonamidas

VS=O 1325 cm⁻¹ e 1125 cm⁻¹ (forte)

VN-H 3350 e 3250 cm⁻¹

δNH- 1550 cm⁻¹

ABSORÇÕES DE COMPOSTOS SULFURADOS

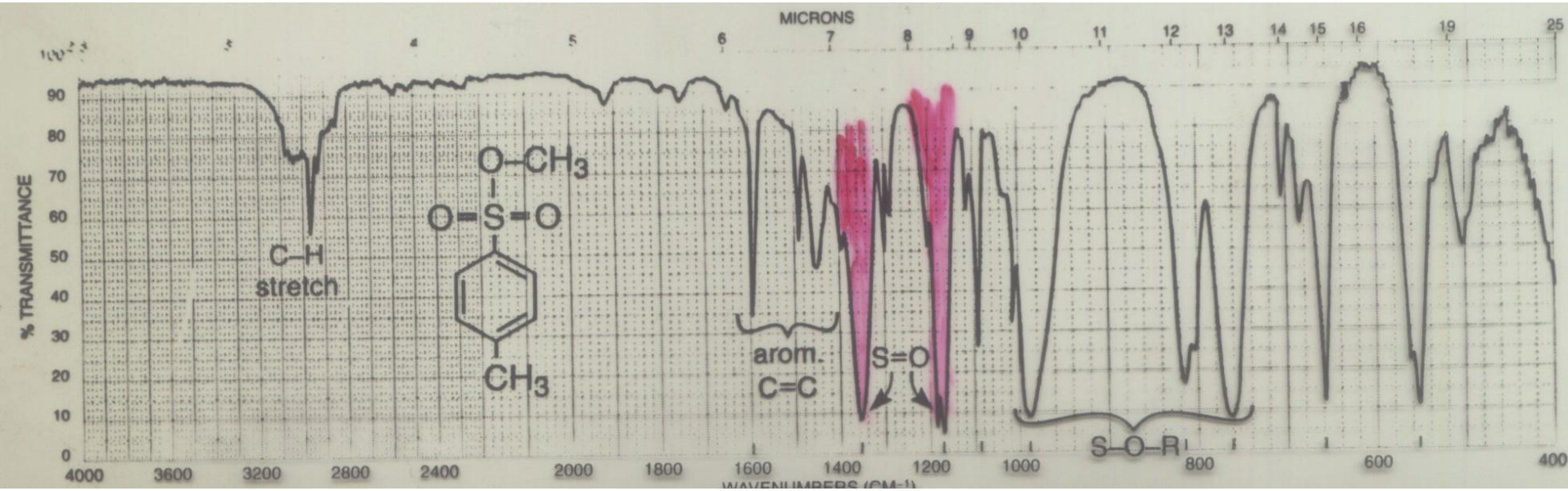


Cloreto de sulfonila

VS=O ass. 1375 cm⁻¹ (forte)

sim 1185 cm⁻¹ (forte)

ABSORÇÕES DE COMPOSTOS SULFURADOS



Sulfonato

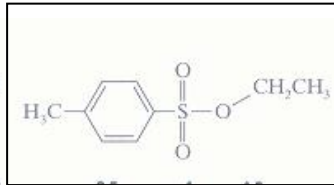
$\nu_{S=O}$ ass. 1350 cm⁻¹ (forte)

sim. 1175 cm⁻¹ (forte)

ν_{S-O-C} 1000 – 750 cm⁻¹ (várias bandas fortes)

ABSORÇÕES DE COMPOSTOS SULFURADOS

10425-6 CAS [80-40-0]
Ethyl *p*-toluenesulfonate

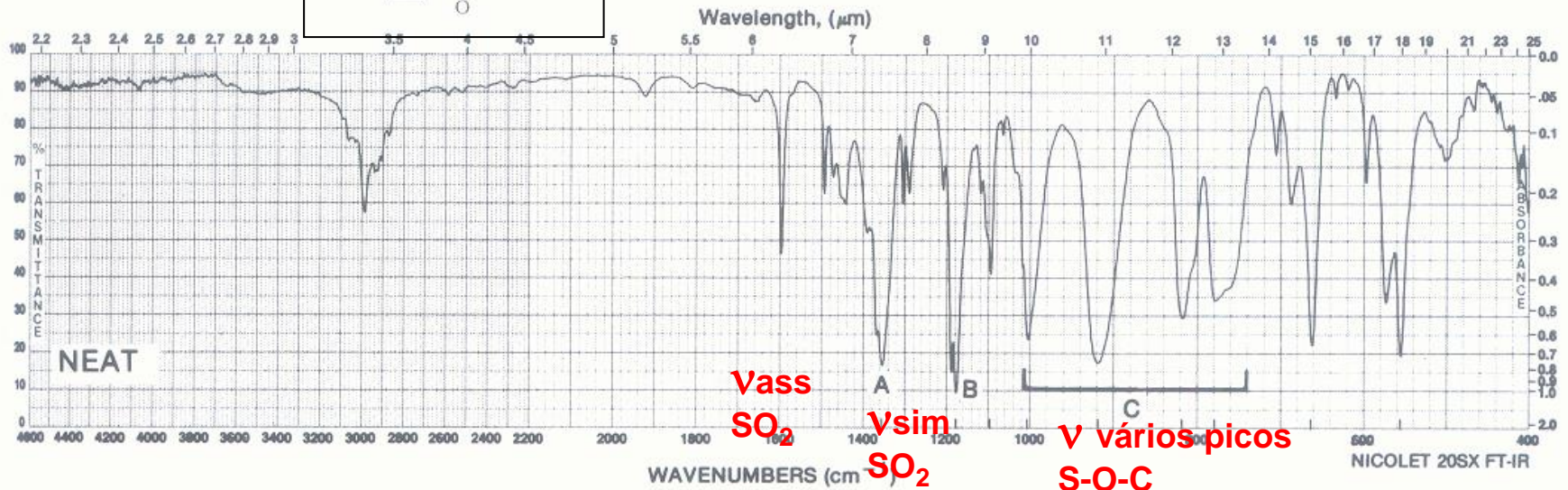


FW 200.26
mp 32-34°C
bp 162°C/10mm

d 1.174
Fp 316°F
n_D 1.5110

IR III, 1166C
NMR II, 2,831D
Merck 10,3805

1355.5	1005.4	778.3
1177.4	918.4	662.5
1095.2	817.1	555.3



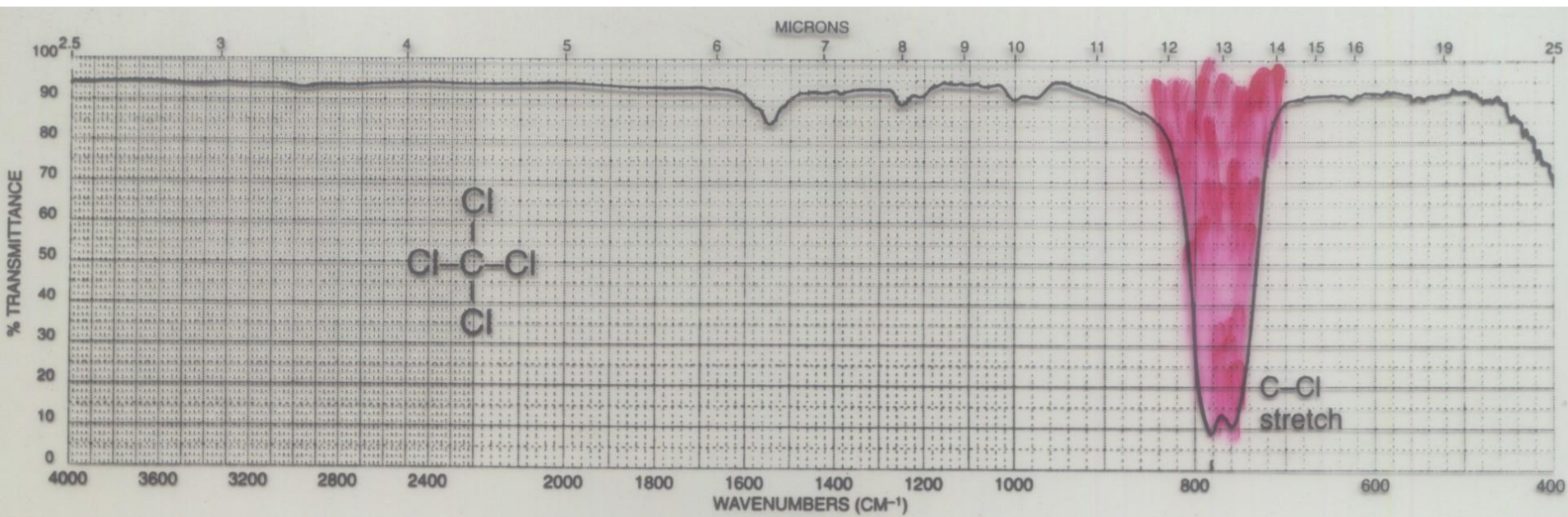
Sulfonato

V_{S=O} ass. 1350 cm⁻¹ (forte)

sim. 1175 cm⁻¹ (forte)

V_{S-O-C} 1000 – 750 cm⁻¹ (várias bandas fortes)

ABSORÇÕES DE HALETOS DE ALQUILA E ARIILA

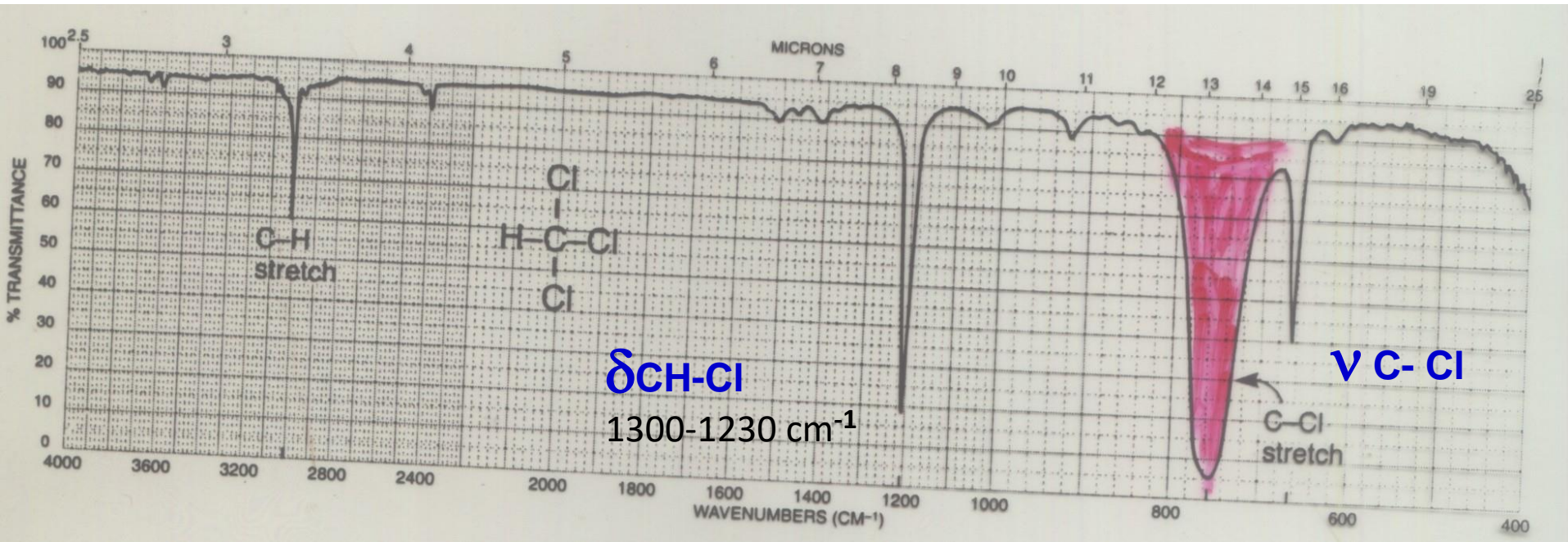


V C-Cl (forte)

alifáticos – 785-540 cm⁻¹

aromáticos – 1096-1089 cm⁻¹

ABSORÇÕES DE HALETOS DE ALQUILA

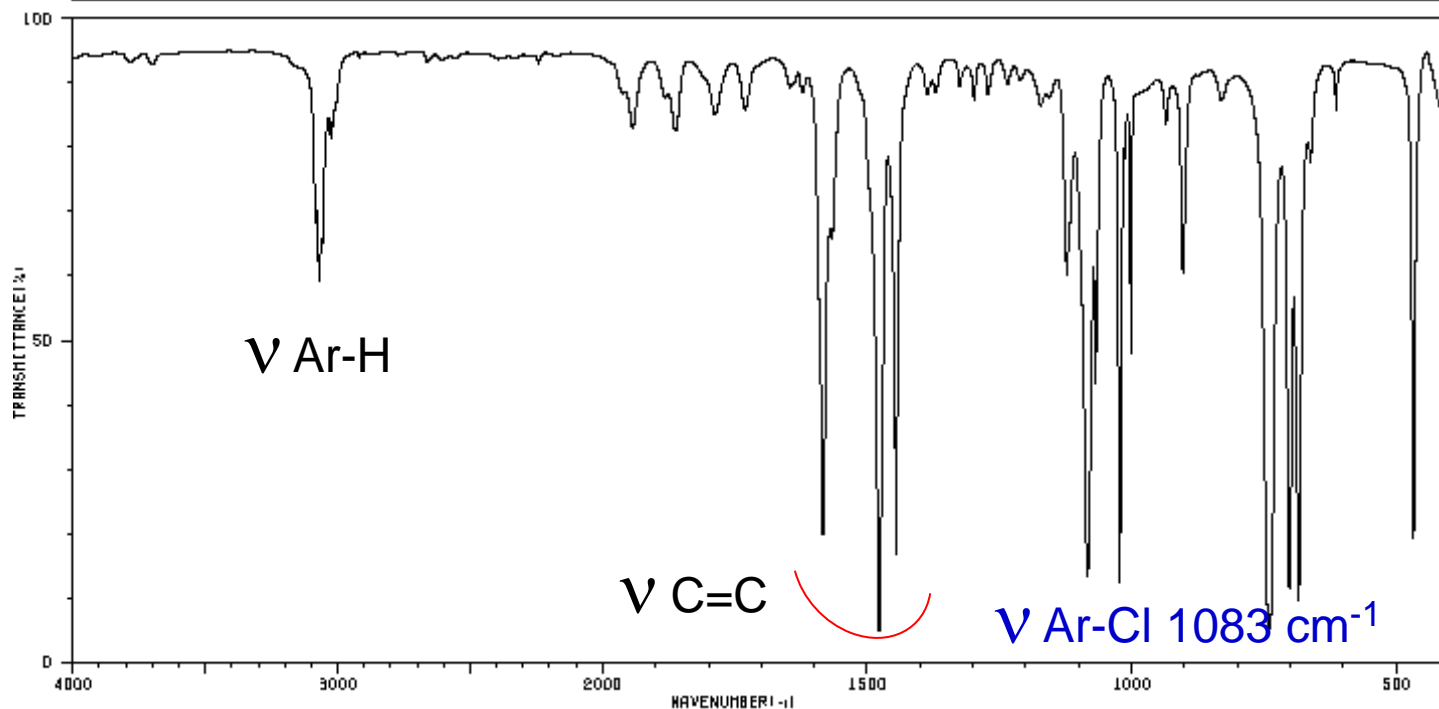


ν C-Cl (forte)

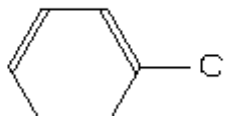
alifáticos – 785-540 cm⁻¹

ABSORÇÕES DE HALETOS DE ARILA

HIT-NO=1734	SCORE= ()	SDBS-NO=2109	IR-NIDA-05126 : LIQUID FILM
CHLOROBENZENE			
C ₆ H ₅ CL			



3084	66	1878	84	1478	4	1083	19	831	84
3070	57	1862	79	1446	16	1068	42	740	5
3059	82	1788	81	1298	84	1023	12	702	10
3026	79	1730	81	1273	84	1013	74	686	9
3016	79	1622	84	1172	84	1002	46	662	74
1956	84	1584	18	1163	84	935	81	614	61
1943	79	1566	62	1123	68	903	68	468	18



ABSORÇÕES DE CLORETOS DE ACILA

