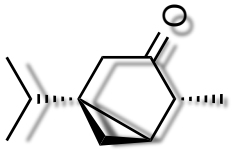
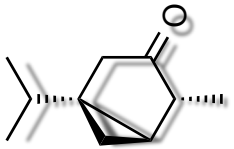


Chemistry 2600

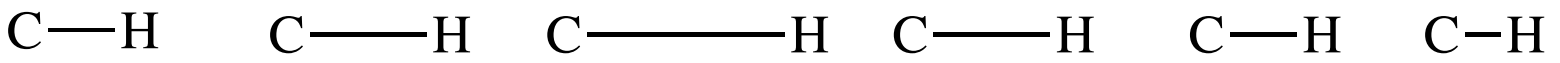
Chapter 14

Infrared Spectroscopy

Infrared Spectroscopy



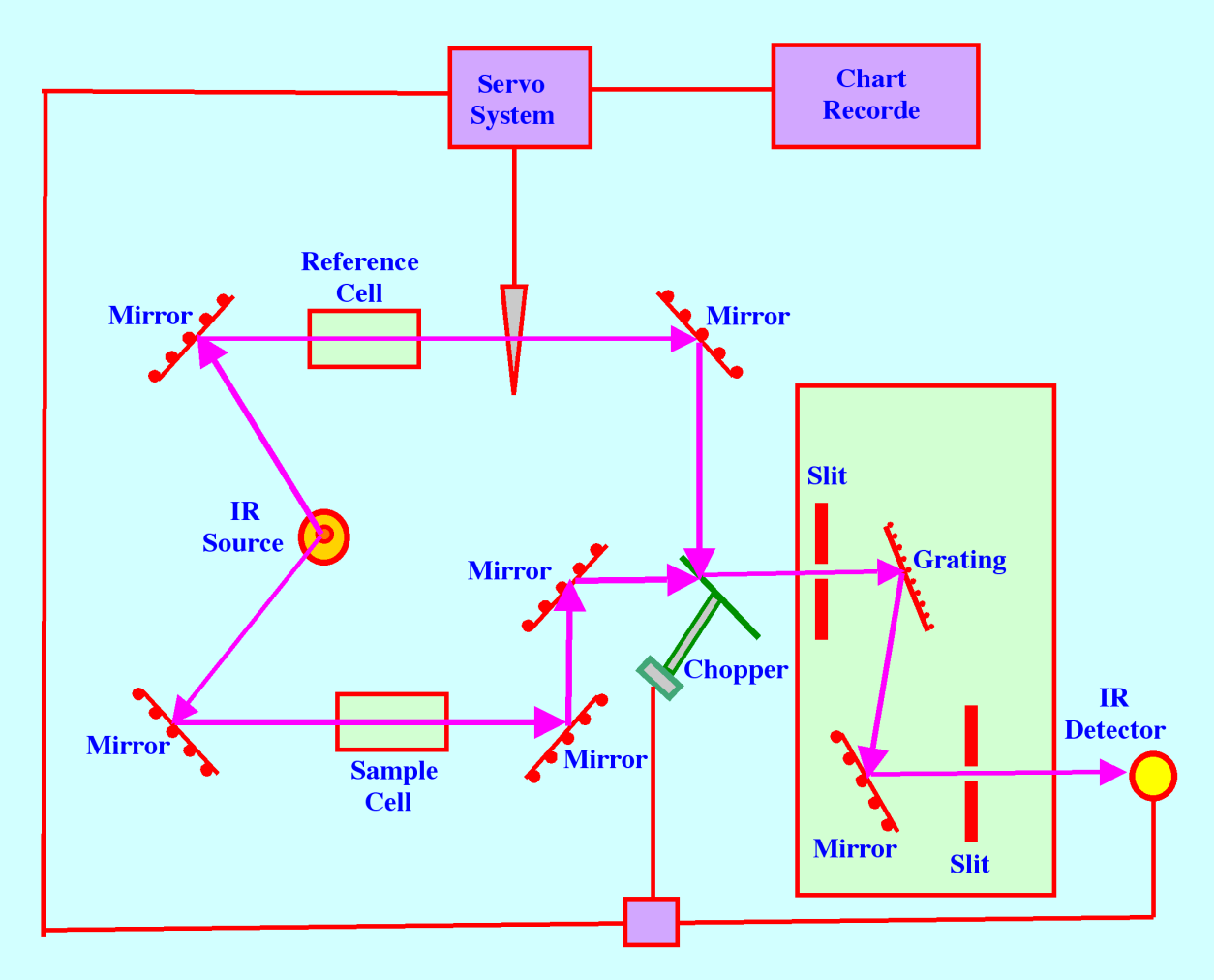
Infra-red Spectroscopy - Good vibrations



These states are quantized.
For absorption to occur, the energy of the photon must exactly match the energy difference between the two states.

IR spectrometers measure the amount of energy transmitted (transmittance) and the wavelength of light absorbed.

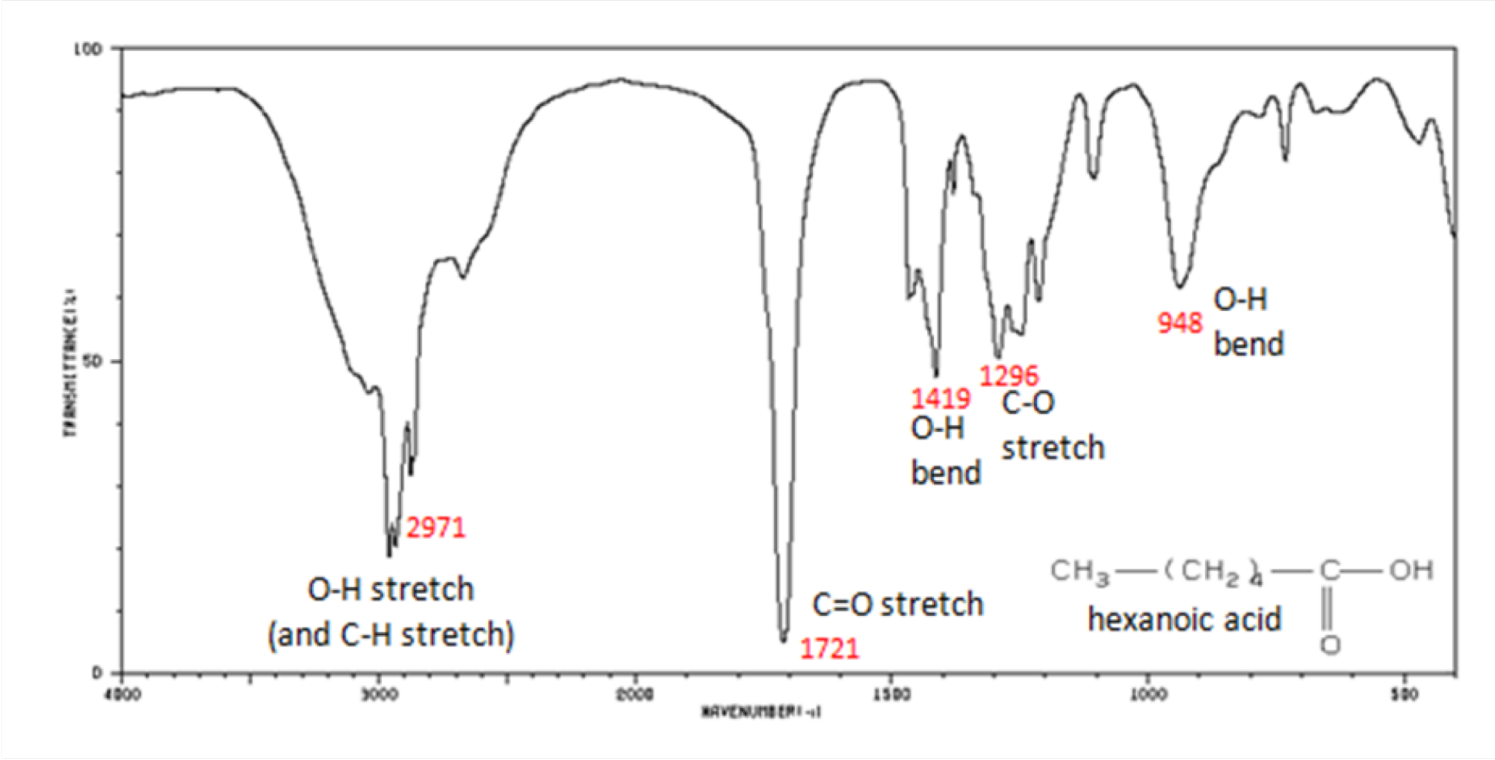
Infrared Spectroscopy



Infrared Spectroscopy

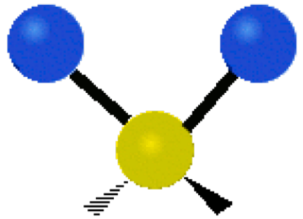
By convention, IR spectra plot transmittance against wavenumber, $\bar{\nu}$ where

$$\bar{\nu} = \frac{1}{\lambda} \quad \text{cm}^{-1} \text{ or wavenumbers}$$

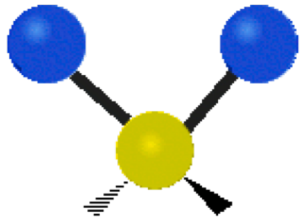


Infrared Spectroscopy

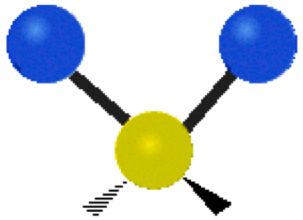
There are many different type of IR ‘modes’. To appear in an IR spectrum, the mode must involve a dipole change.



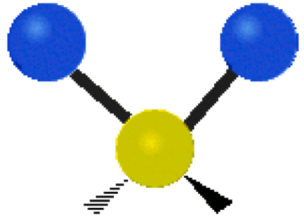
symmetric stretch



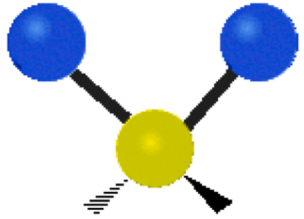
scissor



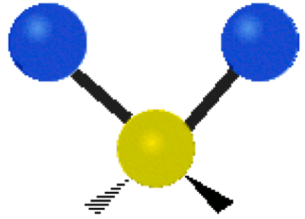
wag



asymmetric stretch

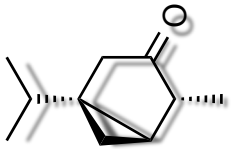


rock



twist

Infrared Spectroscopy



$$\bar{\nu} = \frac{1}{2\pi c}\sqrt{\frac{K}{\mu}} \qquad \mu = \frac{m_1 m_2}{m_1 + m_2}$$

The masses of the atoms.
K is the force constant.

So, the position of an IR band depends on ...

the bond strength.

C≡C	C=C	C—C
2150 cm^{-1}	1650 cm^{-1}	1200 cm^{-1}

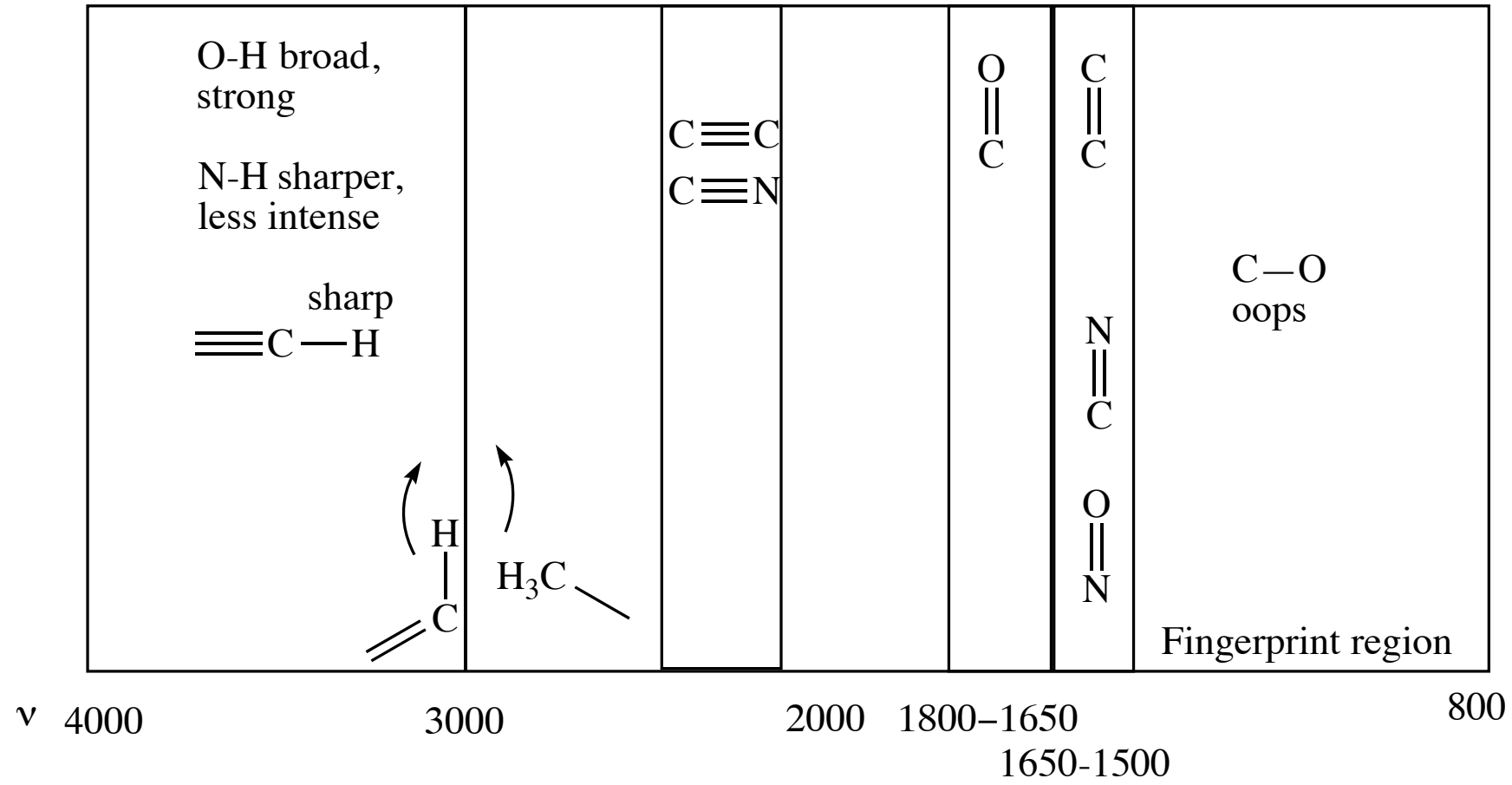
C≡C—H	C=C(H)—H	C—C(H$_2$)—H
3300cm^{-1}	Just above 3000 cm^{-1}	Just below 3000 cm^{-1}

and the masses...

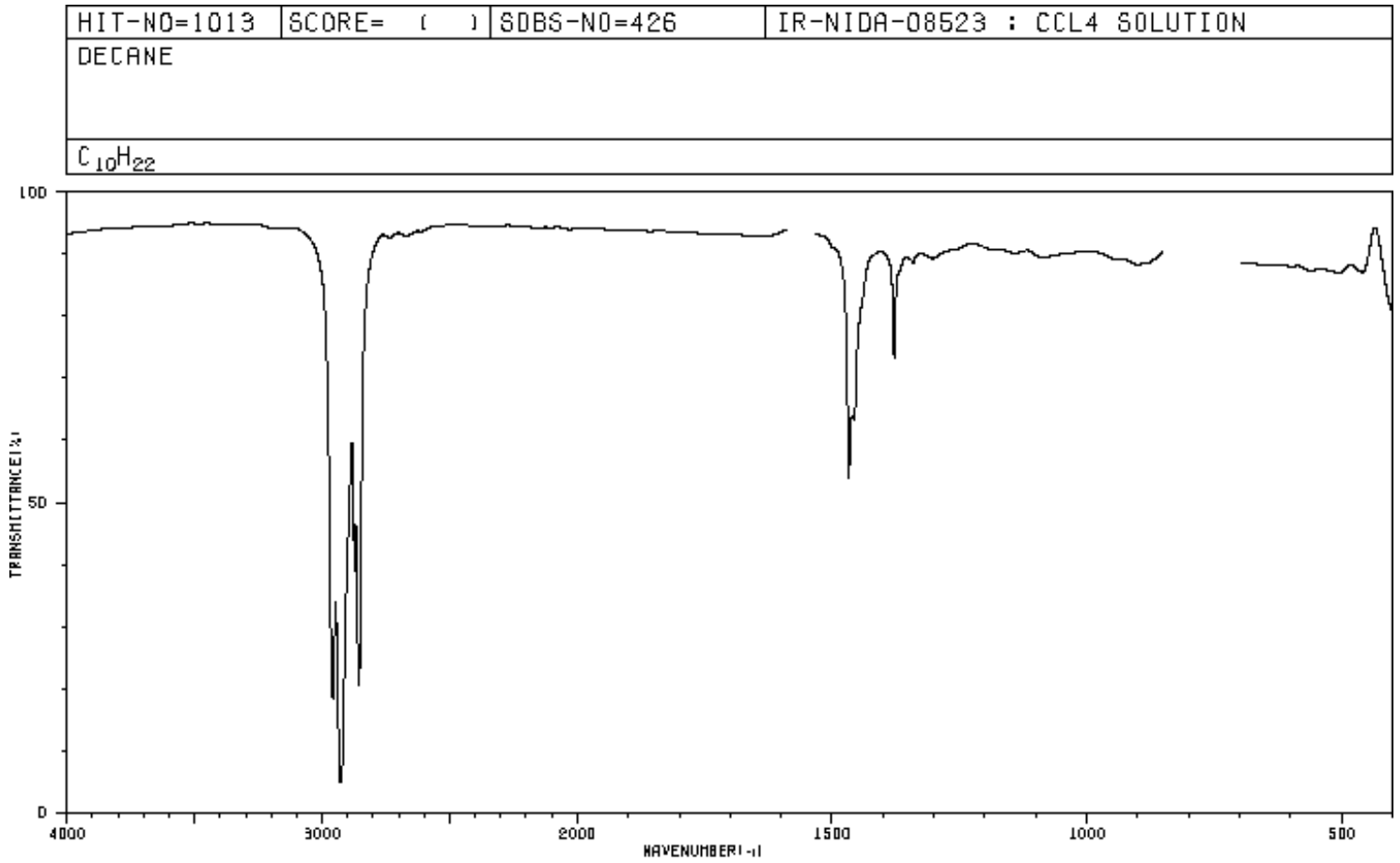
C—H	C—D	C—C	C—O
Just below 3000 cm^{-1}	2200	1200	1100

Infrared Spectroscopy

Getting the most out of an IR in 30 seconds.

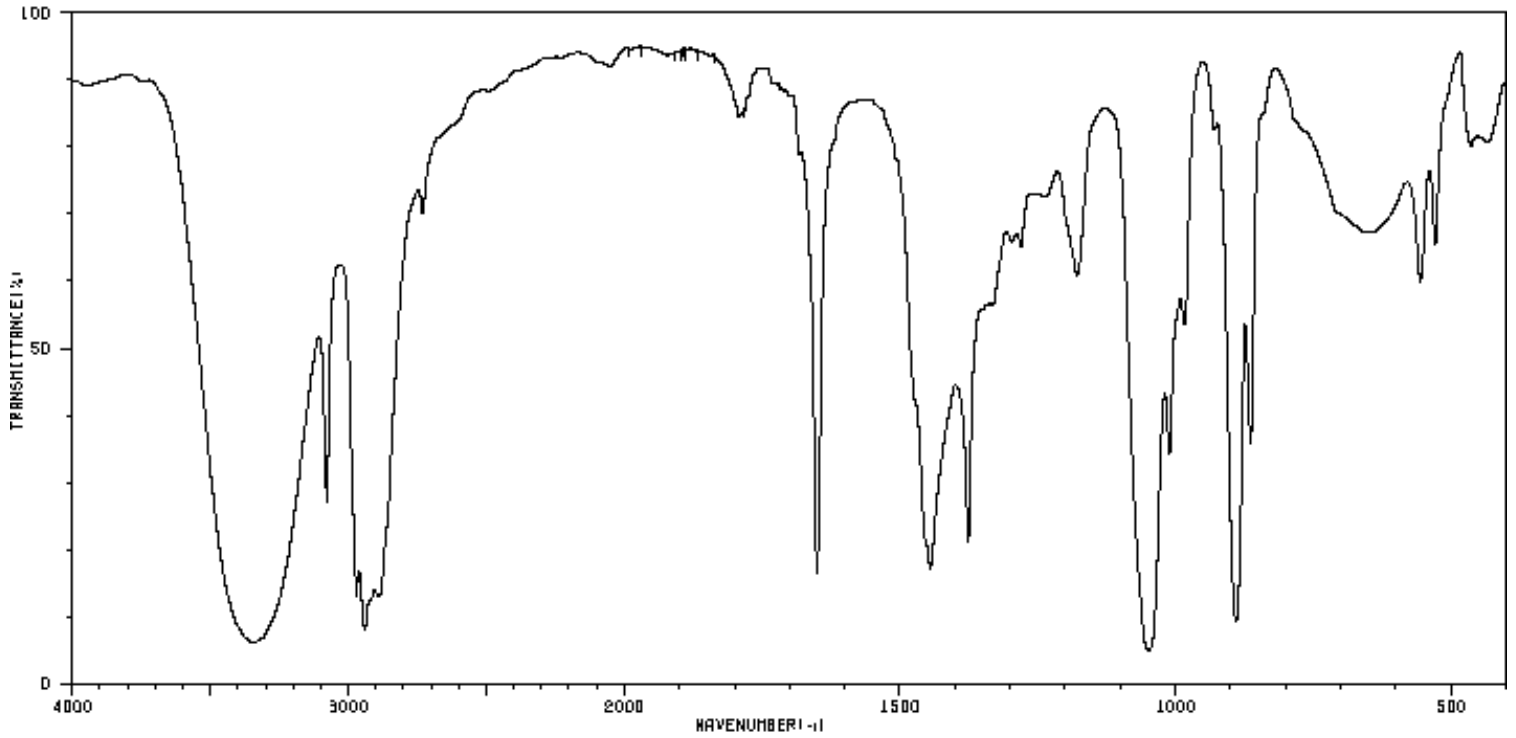


Infrared Spectroscopy - Examples

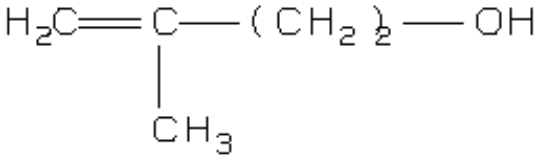


Infrared Spectroscopy - Examples

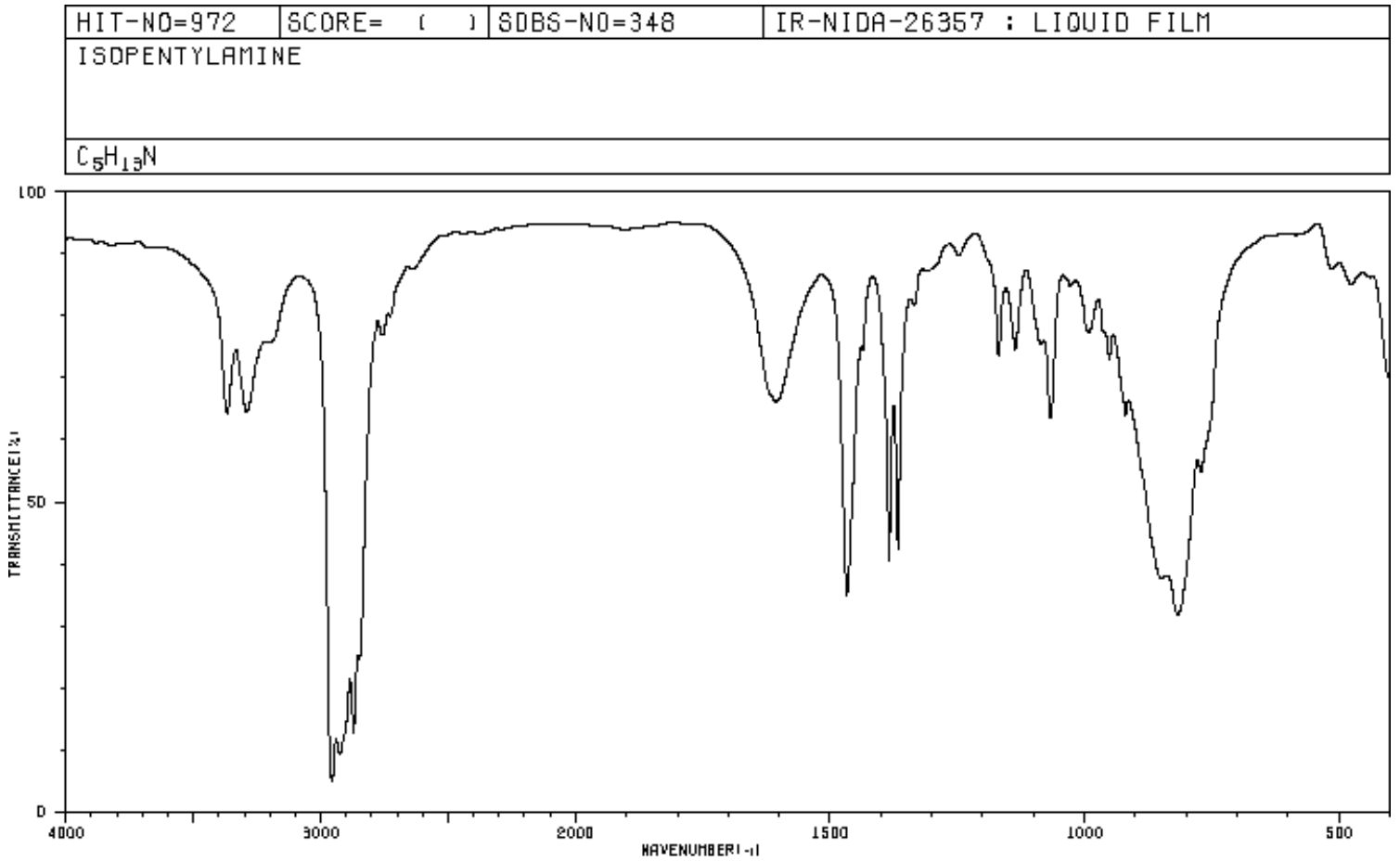
HIT-NO=3965	SCORE= ( )	SDBS-NO=10050	IR-NIDA-02157 : LIQUID FILM
3-METHYL-3-BUTEN-1-OL			
$C_5H_{10}O$			



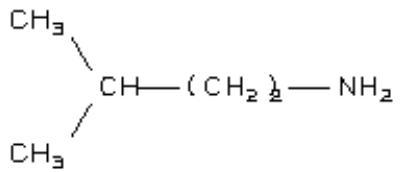
3343	6	2730	68	1298	64	864	34
3333	6	1793	81	1281	62	649	64
3078	26	1785	81	1179	58	556	57
2970	12	1780	84	1049	4	529	62
2940	7	1651	15	1011	33	464	77
2919	12	1445	16	983	52		
2905	13	1376	20	890	8		



Infrared Spectroscopy - Examples



3367	62	1468	39	1081	72	476	81
3289	62	1384	38	1067	60		
2955	4	1367	41	992	74		
2926	0	1336	79	961	70		
2870	12	1248	86	920	62		
2761	74	1169	70	817	30		
1606	64	1136	72	771	62		

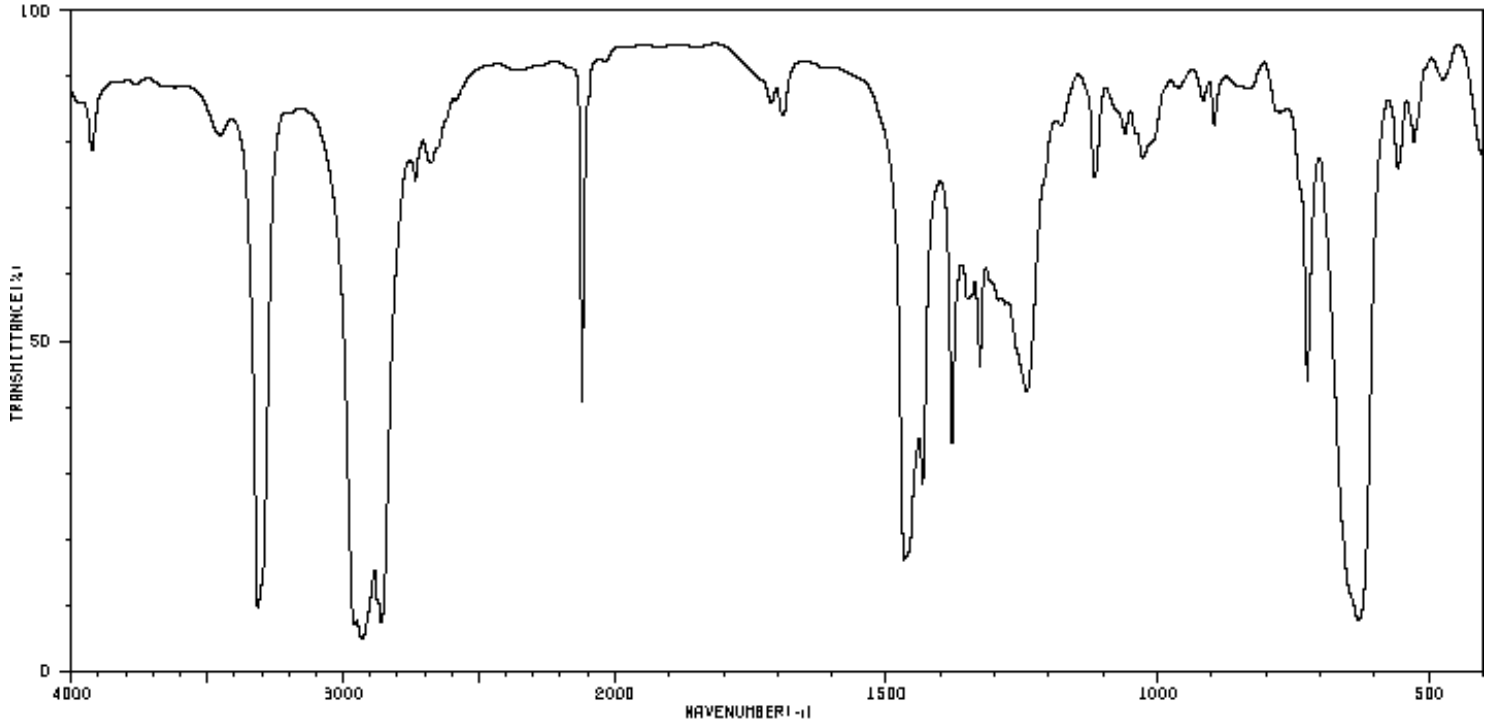


Infrared Spectroscopy - Examples

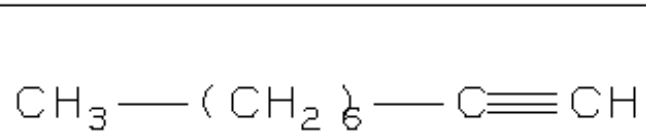
HIT-NO=3147	SCORE= ( )	SDBS-NO=5885	IR-NIDA-09251 : LIQUID FILM

1-NONYNE

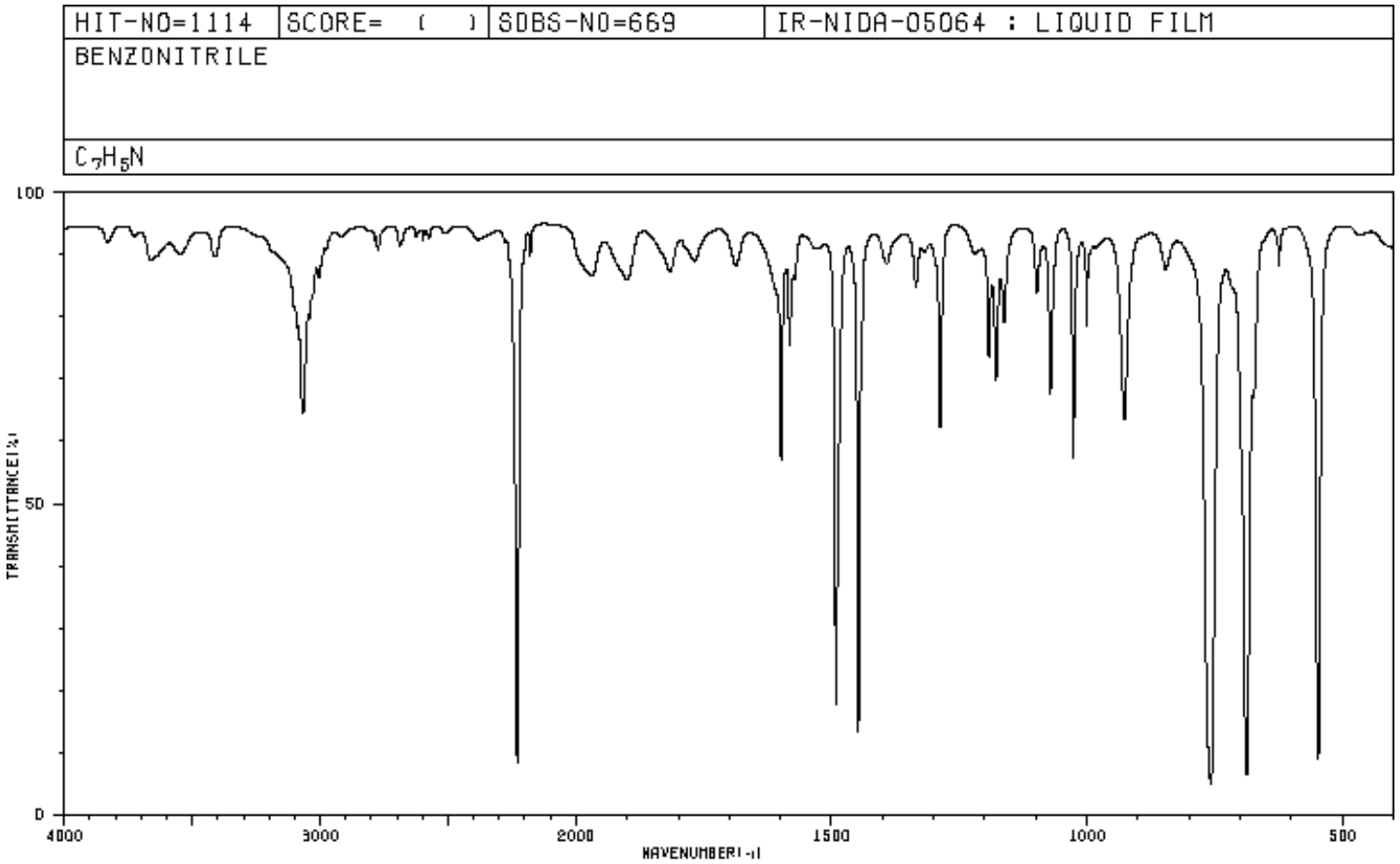
C_9H_{16}



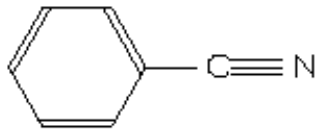
3924	77	2733	72	1468	16	1116	72	896	79
3453	79	2676	74	1433	27	1060	79	838	84
3314	9	2121	36	1379	33	1027	74	724	42
2967	6	2097	81	1361	63	1020	77	629	7
2931	4	1711	84	1344	55	1014	77	557	72
2873	9	1702	64	1327	44	962	64	550	79
2859	7	1691	81	1241	41	916	84	629	77



Infrared Spectroscopy - Examples

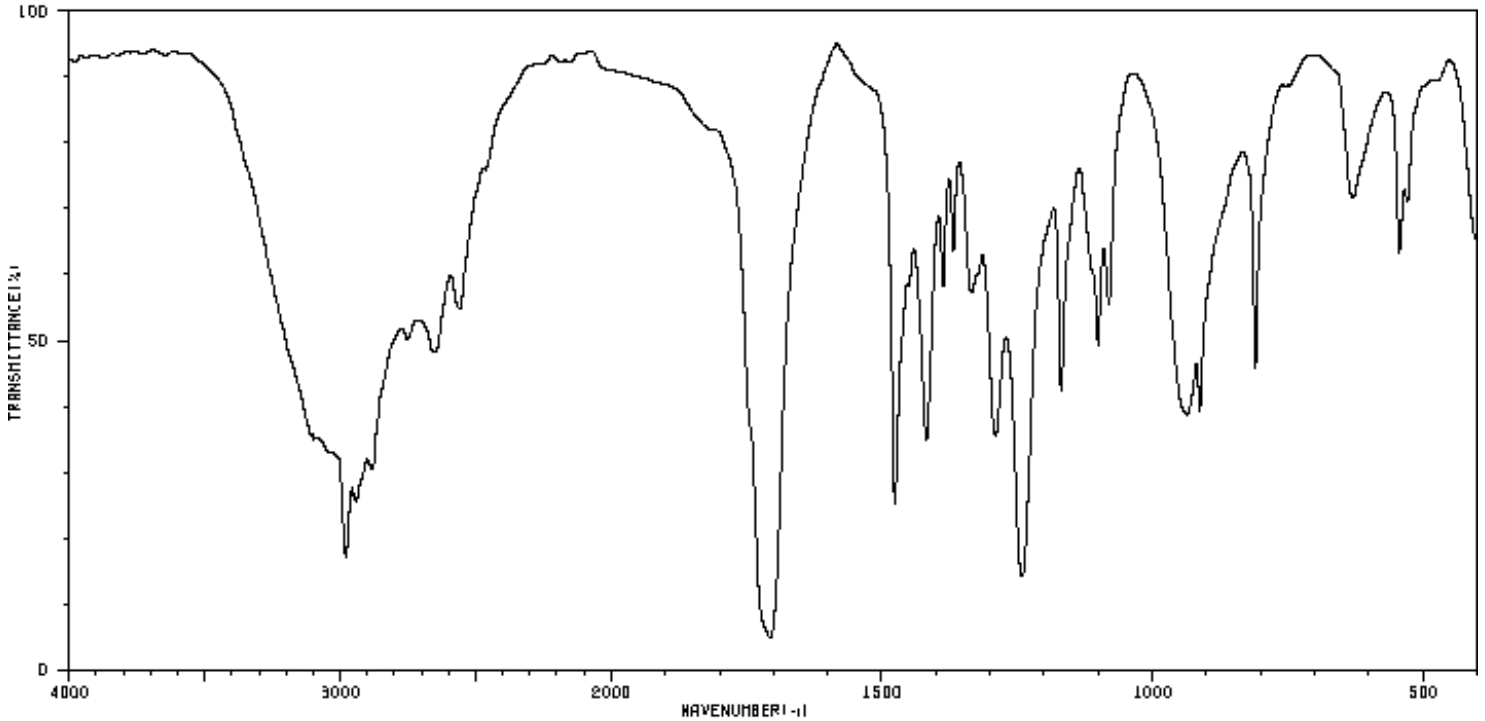


3646	86	2178	86	1682	72	1288	60	1001	74
3412	86	1969	84	1572	81	1193	70	927	60
3088	74	1899	81	1492	17	1178	66	846	64
3066	62	1816	84	1448	12	1163	77	758	4
3004	84	1768	86	1441	72	1098	81	688	6
2256	84	1688	84	1392	84	1072	64	625	64
2230	8	1599	66	1335	81	1027	66	548	8

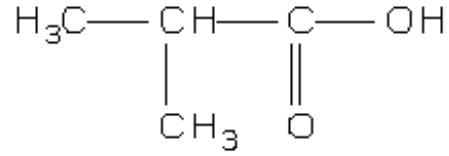


Infrared Spectroscopy - Examples

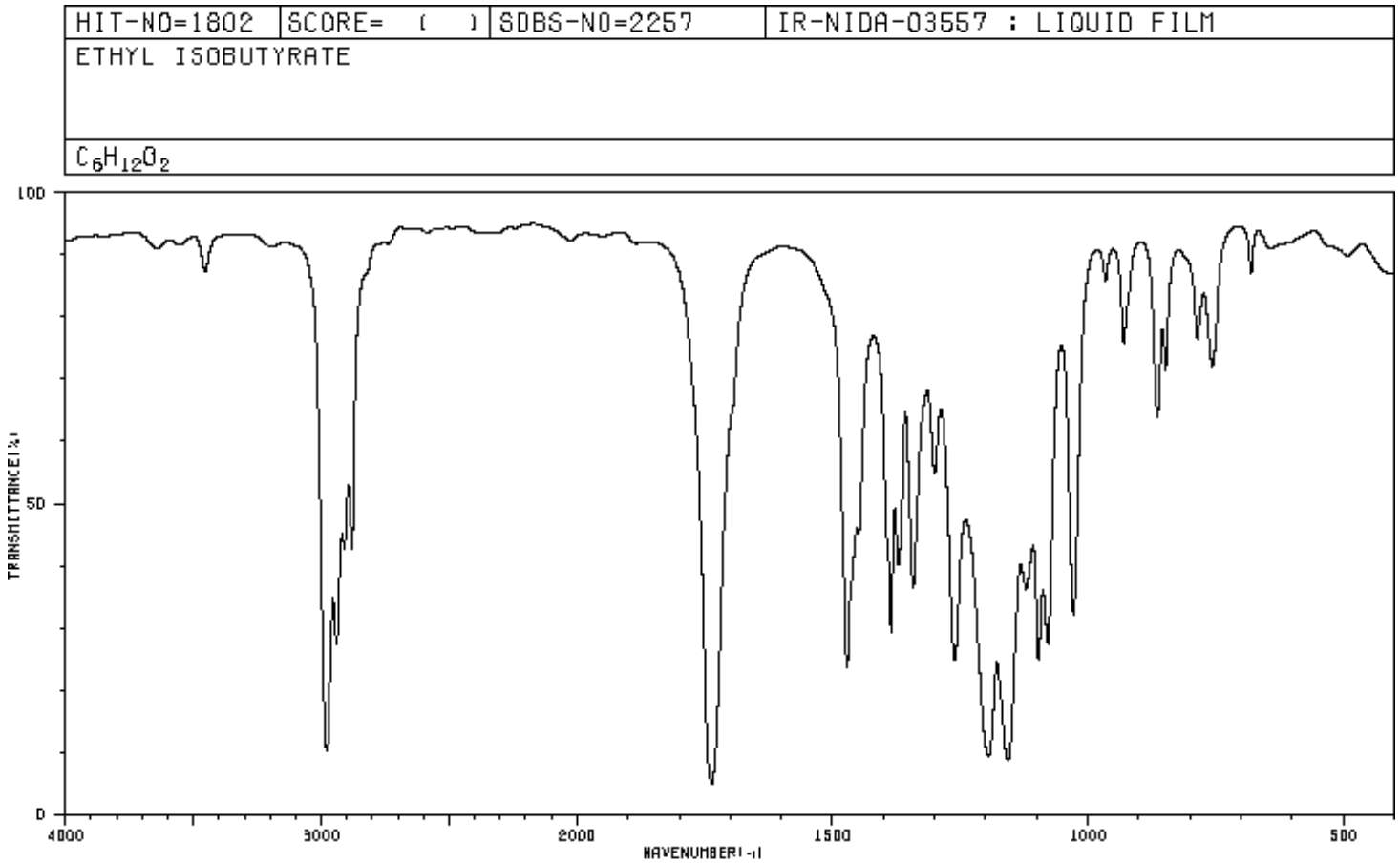
HIT-NO=1319	SCORE= ( )	SDBS-NO=1224	IR-NIDA-58450 : LIQUID FILM
ISOBUTYRIC ACID			
$C_4H_8O_2$			



2979	16	2669	69	1290	34	811	44
2968	21	1707	4	1241	13	630	68
2951	25	1478	24	1169	41	544	60
2940	24	1418	34	1100	47	529	68
2880	29	1387	57	1080	53		
2750	49	1368	60	937	37		
2662	46	1336	66	913	38		



Infrared Spectroscopy - Examples



3466	84	1386	27	1121	35	848	68
2978	9	1372	38	1097	23	786	74
2940	26	1342	35	1079	26	756	70
2910	41	1301	62	1028	31	681	84
2879	41	1261	23	965	81	493	86
1737	4	1195	8	930	72		
1471	22	1167	8	864	62