The C=O stretching frequency

aldehydes and ketones

A summary of the principle infrared bands and their assignments. R is an aliphatic group.

C=O	aldehydes	R(C=O)H	1740-1720	S(sh)	14
	ketones	R(C=O)R	1730-1710	S(sh)	35

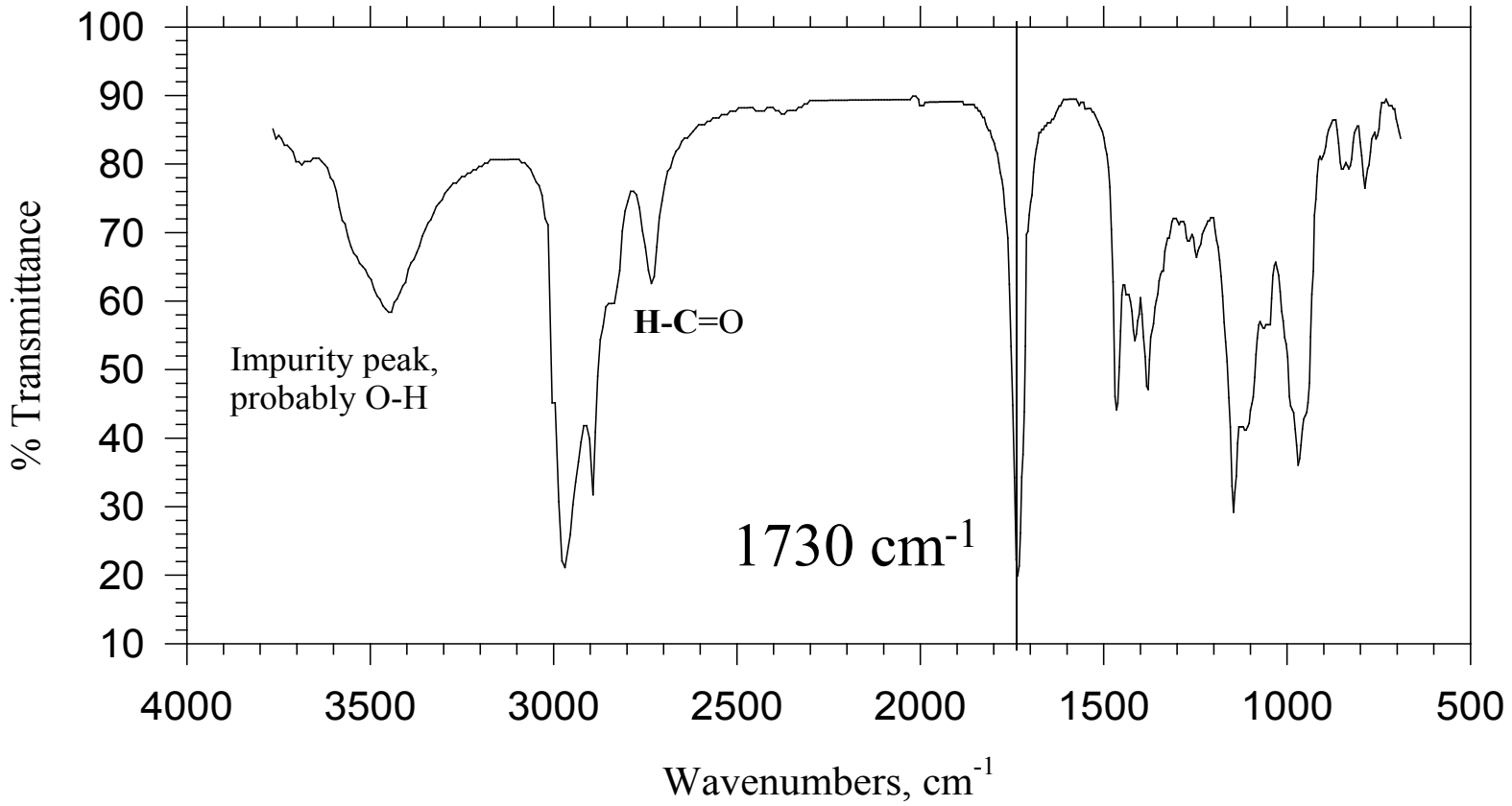


Figure IR-14. Butanal, neat liquid, thin film: $CH_3CH_2CH_2CHO$

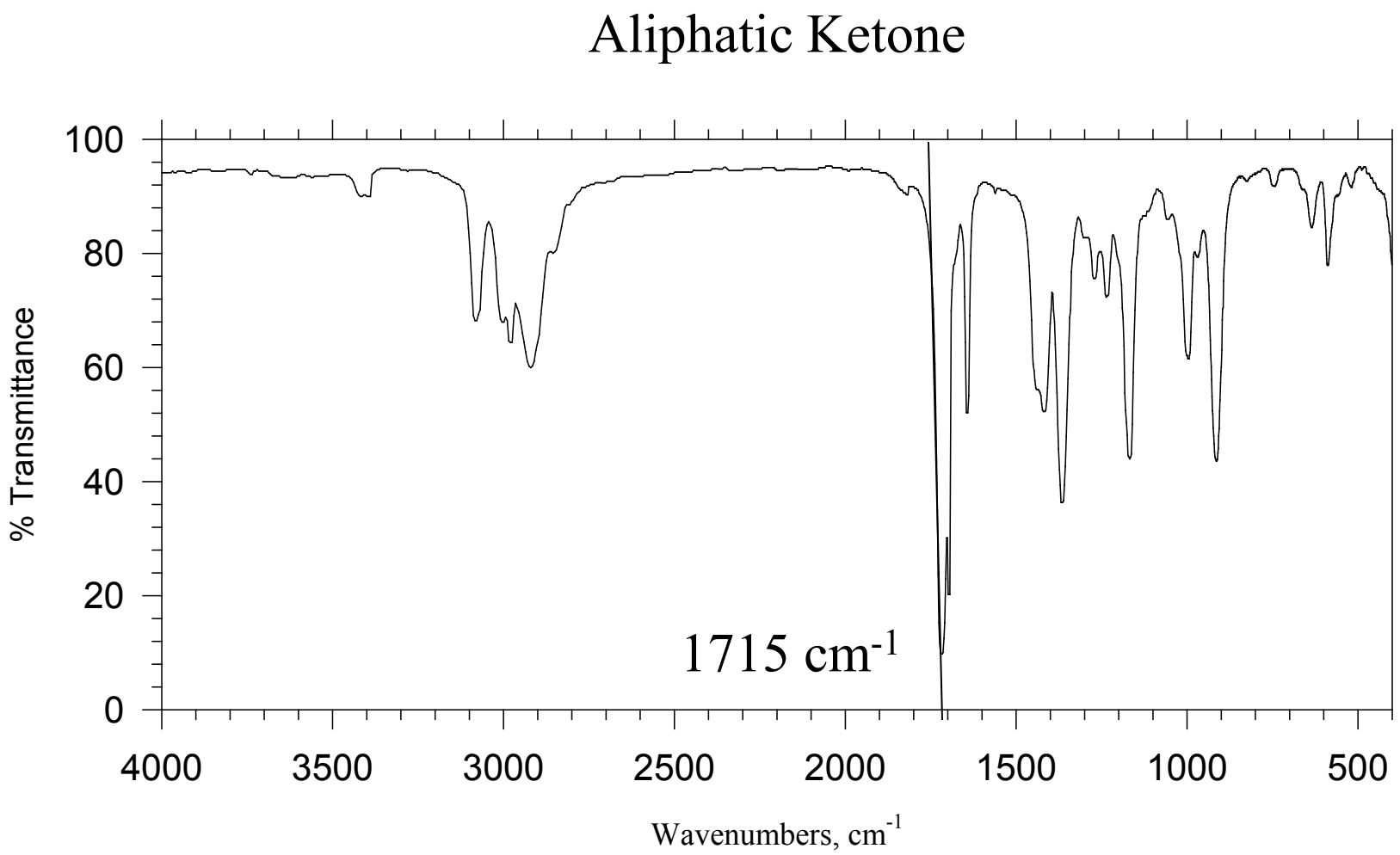


Figure IR-35. 5-Hexene-2-one, neat liquid: $CH_2=CH_2CH_2CH_2COCH_3$

The C=O stretching frequency

esters

A summary of the principle infrared bands and their assignments. R is an aliphatic group.

C=O	aldehydes	R(C=O)H	1740-1720	S(sh)	14
	ketones	R(C=O)R	1730-1710	S(sh)	35
	esters	R(CO_2)R	1750-1735	S(sh)	33, 34

Aliphatic Ester

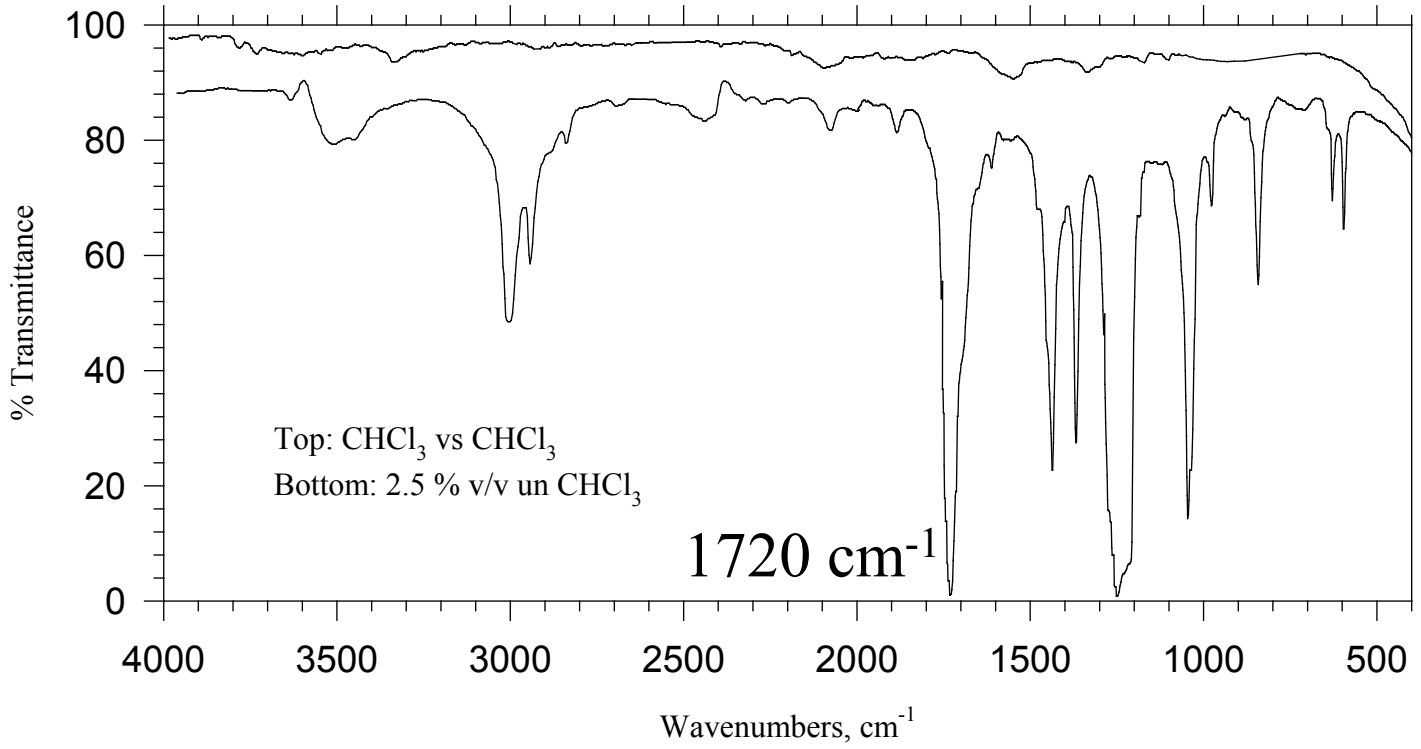
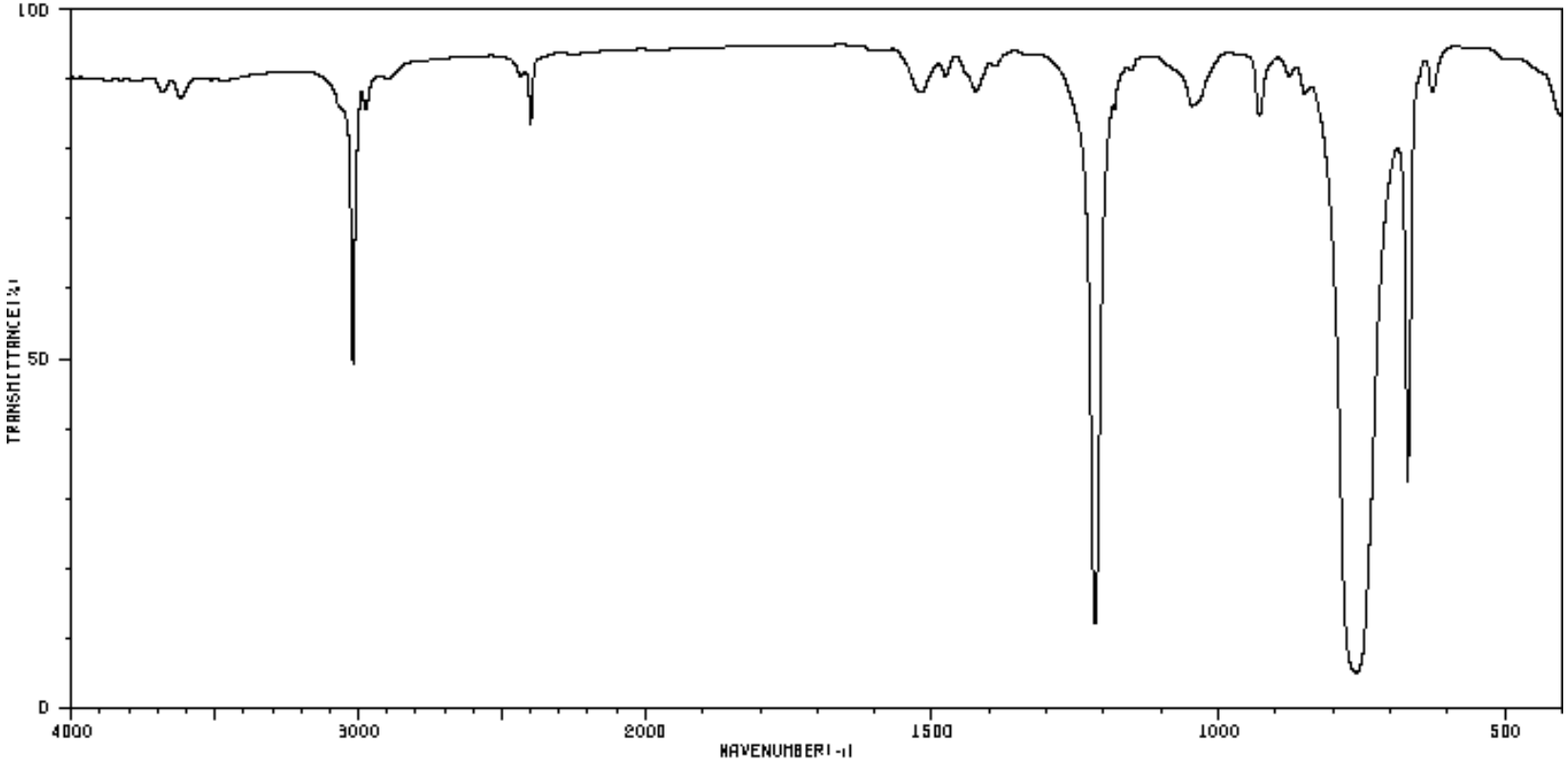


Figure IR-33. Methyl acetate in 0.1 mm NaCl cells: $CH_3CO_2CH_3$

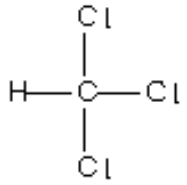
HIT-NO=1233	SCORE= ( )	SDBS-NO=894	IR-NIDA-01674 : LIQUID FILM

CHLOROFORM

$CHCl_3$



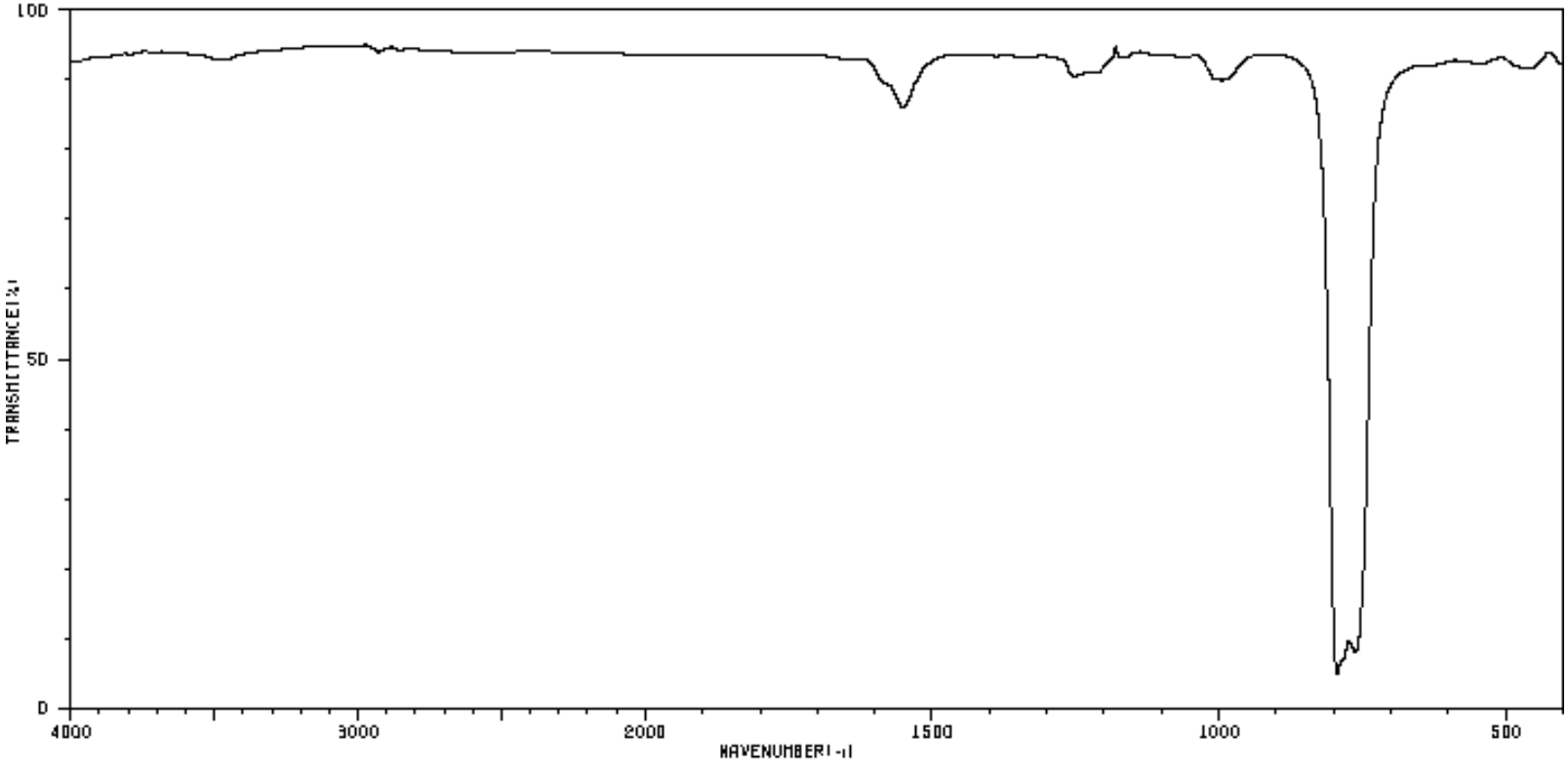
3683	84	1216	11
3618	84	1047	84
3019	47	1041	84
2975	81	929	81
2400	79	760	4
1520	84	671	31
1423	84	627	84



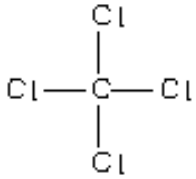
HIT-NO=1394	SCORE= ( )	SDBS-NO=1321	IR-NIDA-06337 : LIQUID FILM

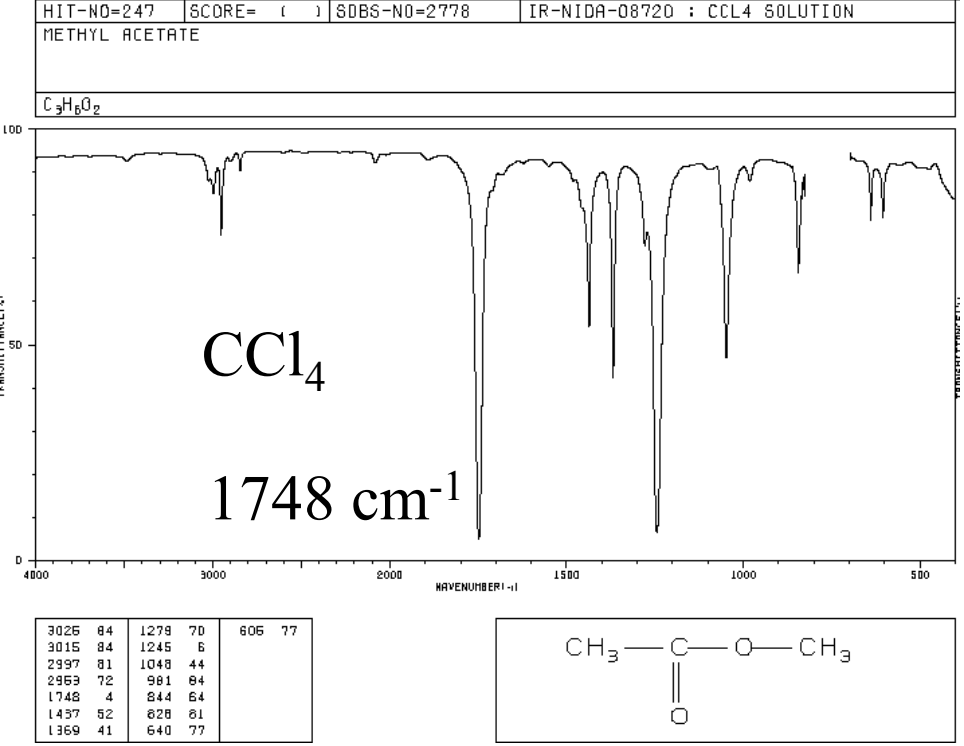
TETRACHLOROMETHANE

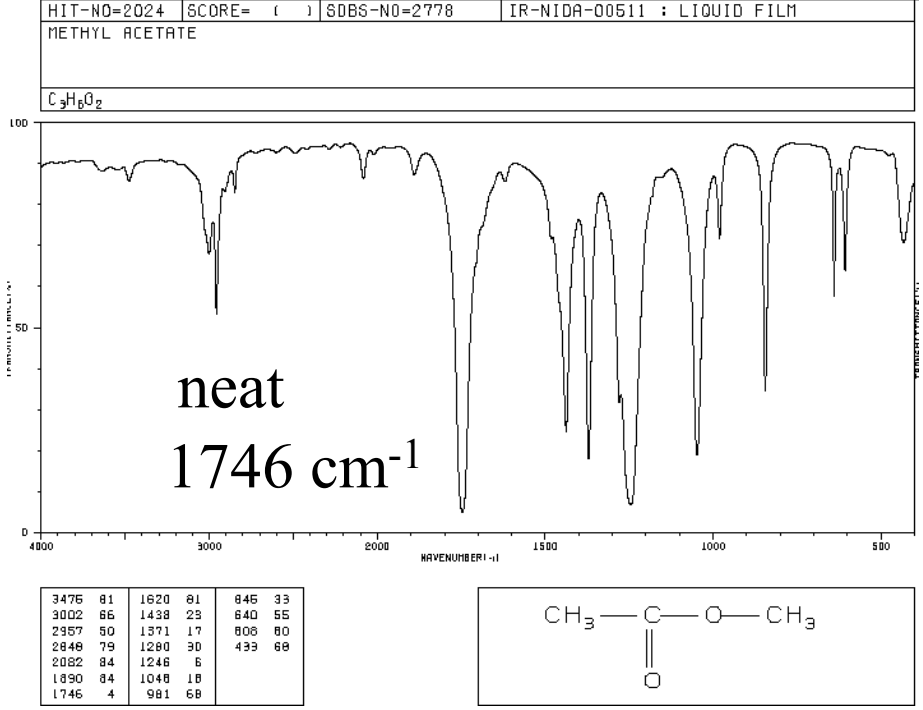
CCL_4

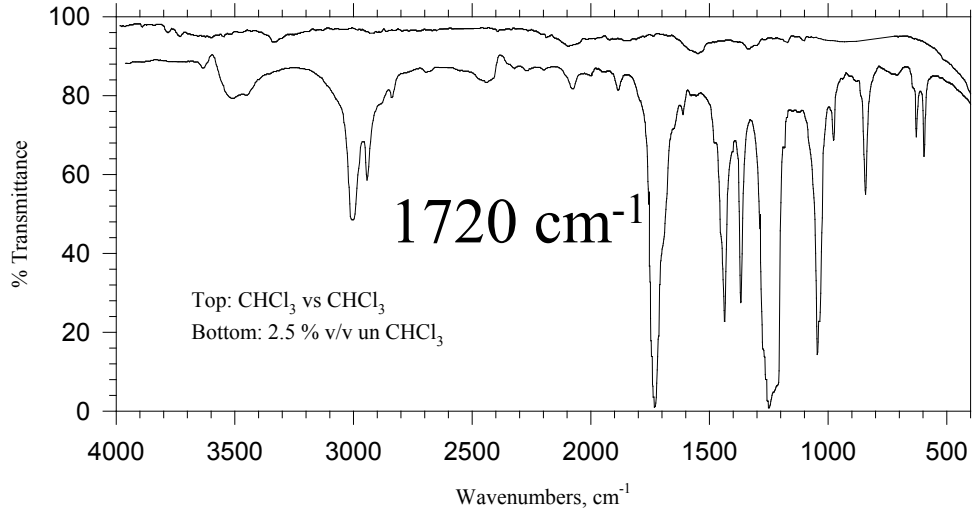


1550	81
994	86
795	4
762	7









methyl acetate
in different
solvents

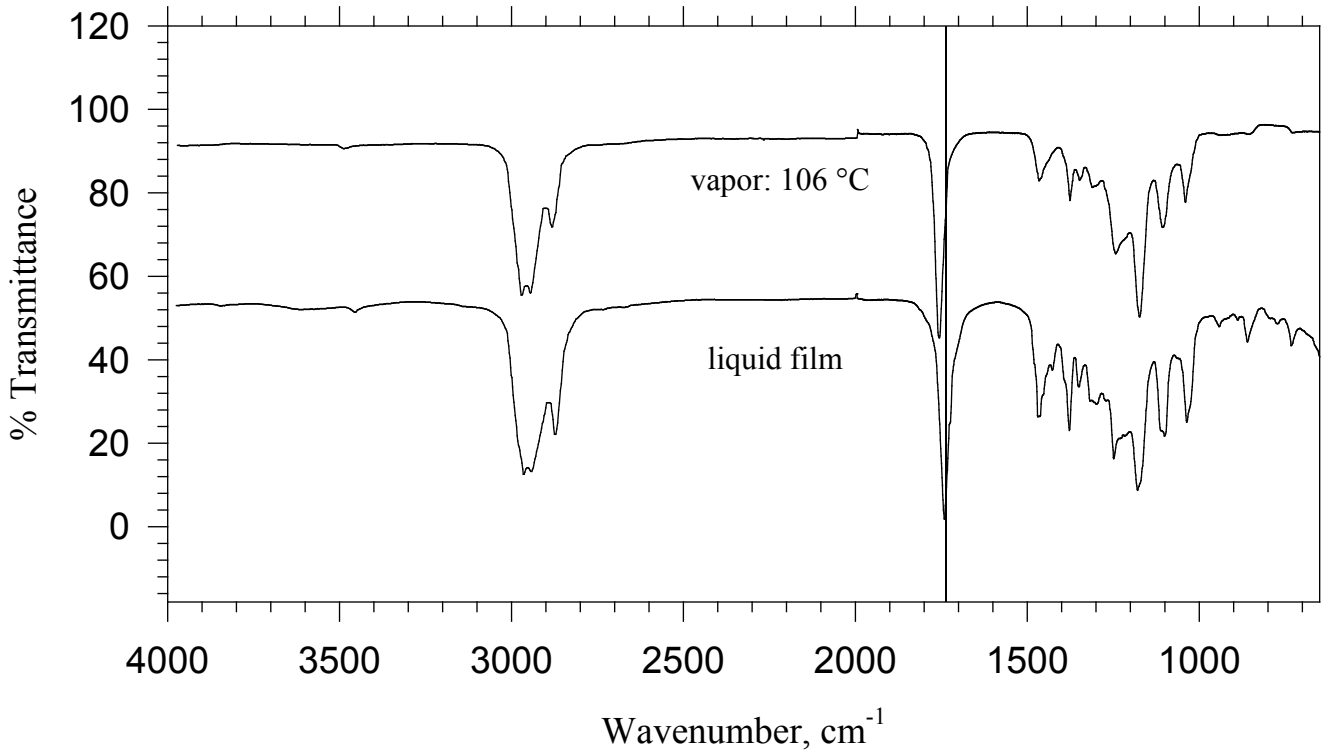


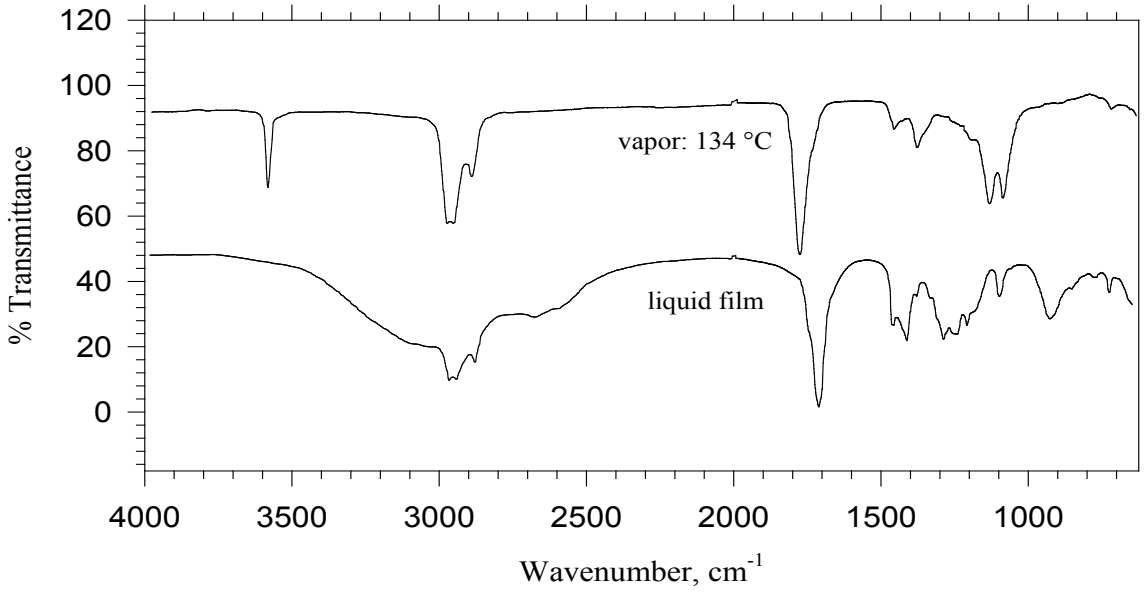
Figure IR-34. Vapor and liquid spectra of ethyl n-hexanoate: $CH_3CH_2CH_2CH_2CH_2CO_2CH_2CH_3$

The C=O stretching frequency

aliphatic acids

A summary of the principle infrared bands and their assignments. R is an aliphatic group.

C=O	aldehydes	R(C=O)H	1740-1720	S(sh)	14
	ketones	R(C=O)R	1730-1710	S(sh)	35
	esters	$R(CO_2)R$	1750-1735	S(sh)	33, 34
	carboxylic acids	RCO_2H	1720-1680	S(sh)	26,27,30



Aliphatic Acid

vapor 1740 cm^{-1}

neat 1710 cm^{-1}

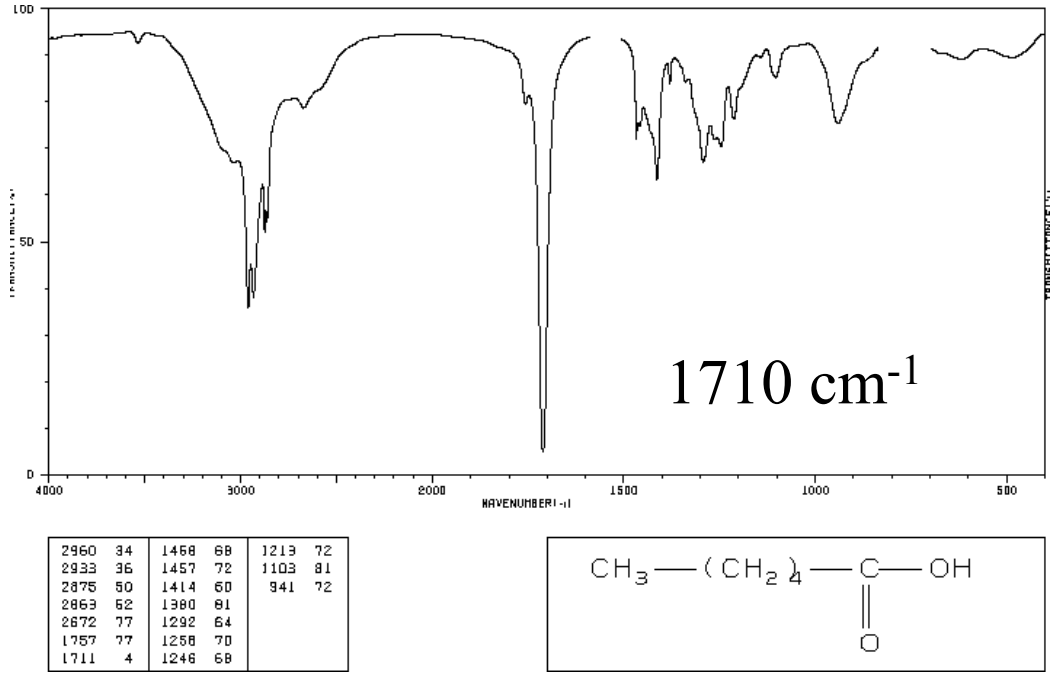


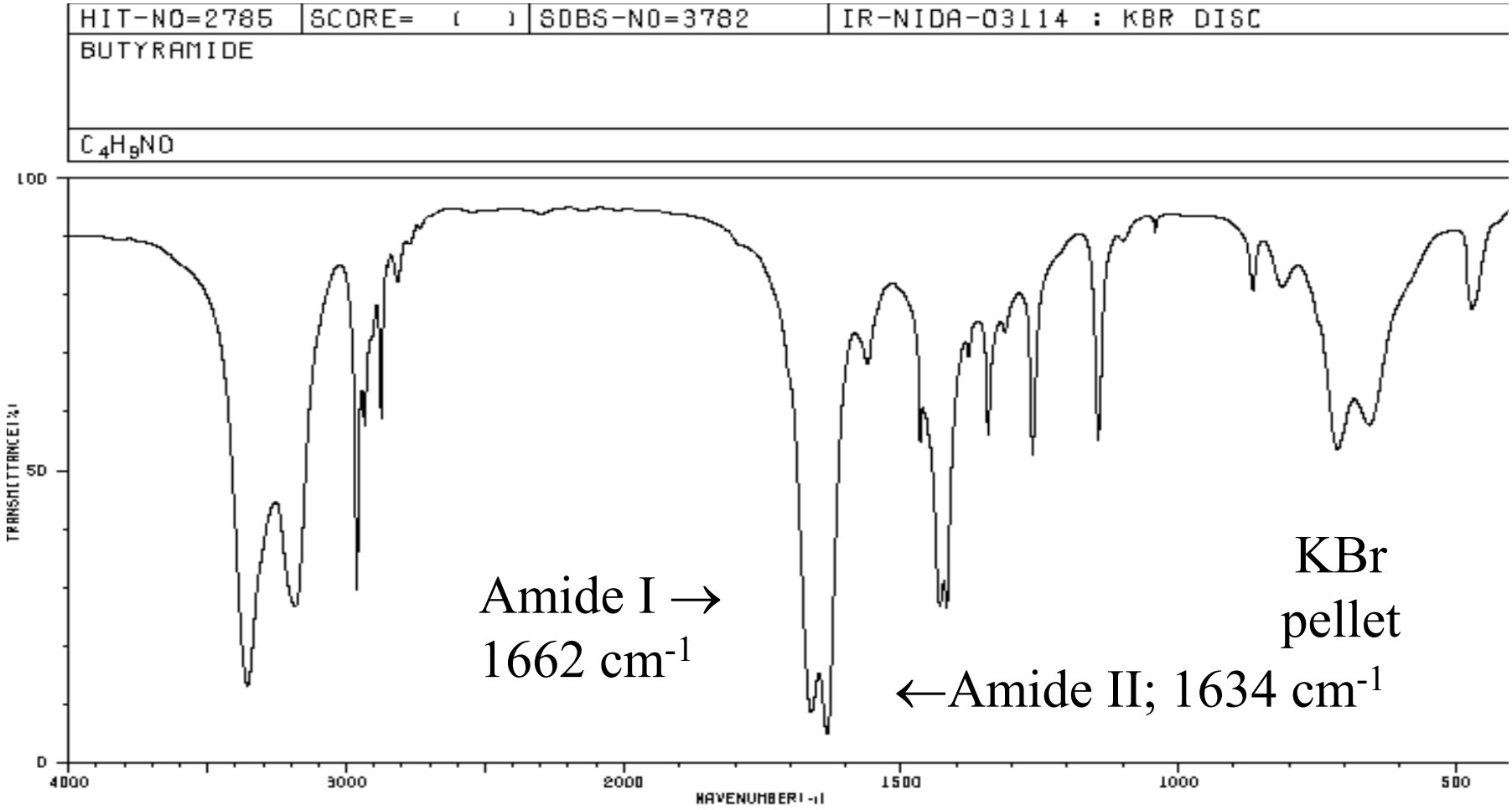
Figure IR-26. The vapor, liquid and CCl_4 soln spectra of hexanoic acid: $CH_3(CH_2)_4\ CO_2H$

The C=O stretching frequency

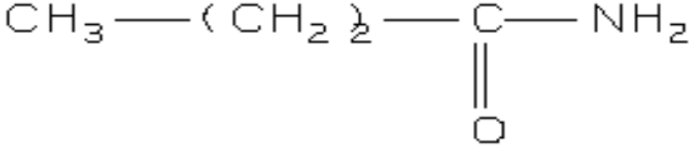
aliphatic amides

A summary of the principle infrared bands and their assignments. R is an aliphatic group.

C=O	aldehydes	R(C=O)H	1740-1720	S(sh)	14
	ketones	R(C=O)R	1730-1710	S(sh)	35
	esters	$R(CO_2)R$	1750-1735	S(sh)	33, 34
	carboxylic acids	RCO_2H	1720-1680	S(sh)	26,27,30
	amides (Amide I)	$RCONH_2$, RCONHR	1670-1640	S(sh)	19, 21
	(Amide II)	$RCONH_2$	1650-1620	S(sh)	19, 21
	(Amide II)	RCONHR	1550	S(sh)	19, 21
	amide	$RCONR_2$	1650-1620	S(sh)	23



3366	12	1634	4	1313	70	666	66
3184	25	1561	66	1263	50	470	74
2962	28	1468	52	1145	53		
2934	66	1430	26	866	77		
2873	57	1418	25	813	79		
2816	79	1379	66	803	79		
1662	8	1344	69	713	62		



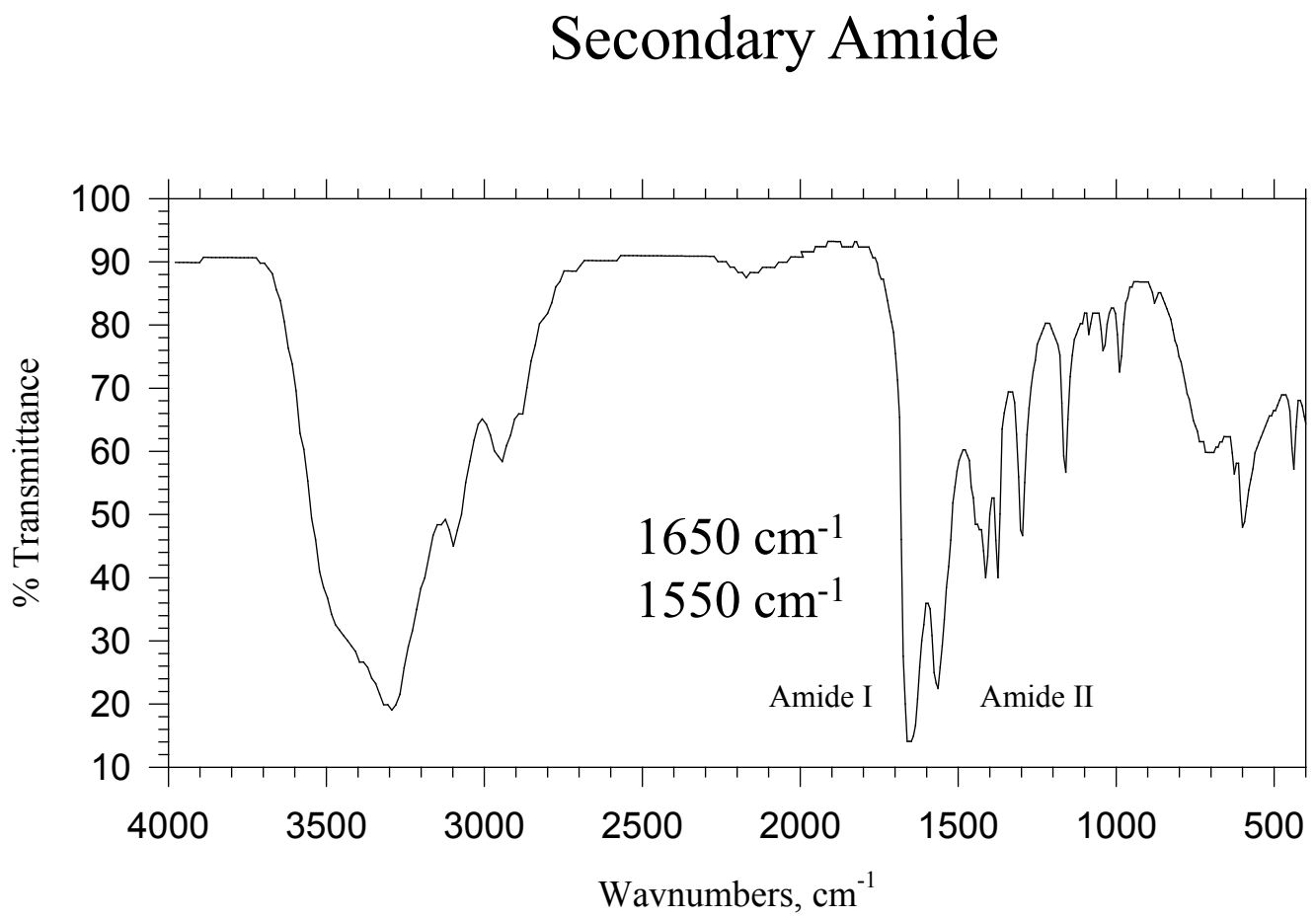


Figure IR-21. N-Methyl acetamide, neat liquid; thin film: $CH_3CONHCH_3$

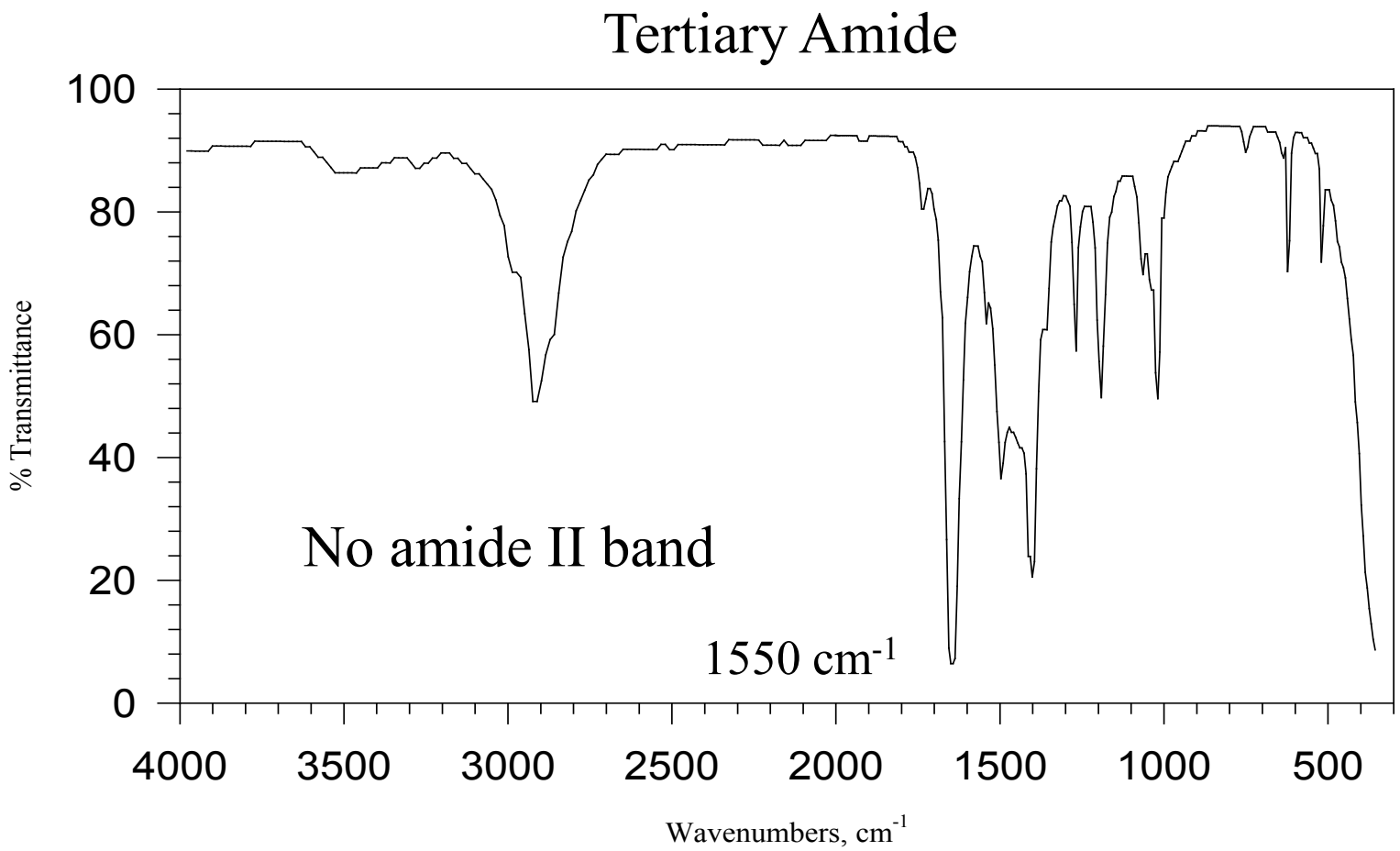


Figure IR-23. N,N-Dimethylacetamide, neat liquid; thin film: $CH_3CON(CH_3)_2$

The C=O stretching frequency

anhydrides

A summary of the principle infrared bands and their assignments. R is an aliphatic group.

C=O	aldehydes	R(C=O)H	1740-1720	S(sh)	14
	ketones	R(C=O)R	1730-1710	S(sh)	35
	esters	R(CO_2)R	1750-1735	S(sh)	33, 34
	carboxylic acids	RCO_2H	1720-1680	S(sh)	26,27,30
	amides (Amide I)	R$CONH_2$, RCONHR	1670-1640	S(sh)	19, 21
	(Amide II)	R$CONH_2$	1650-1620	S(sh)	19, 21
	(Amide II)	RCONHR	1550	S(sh)	19, 21
	amide	R$CONR_2$	1650-1620	S(sh)	23
	anhydrides	R(CO_2CO)R	1820, 1750	S, S(sh)	36

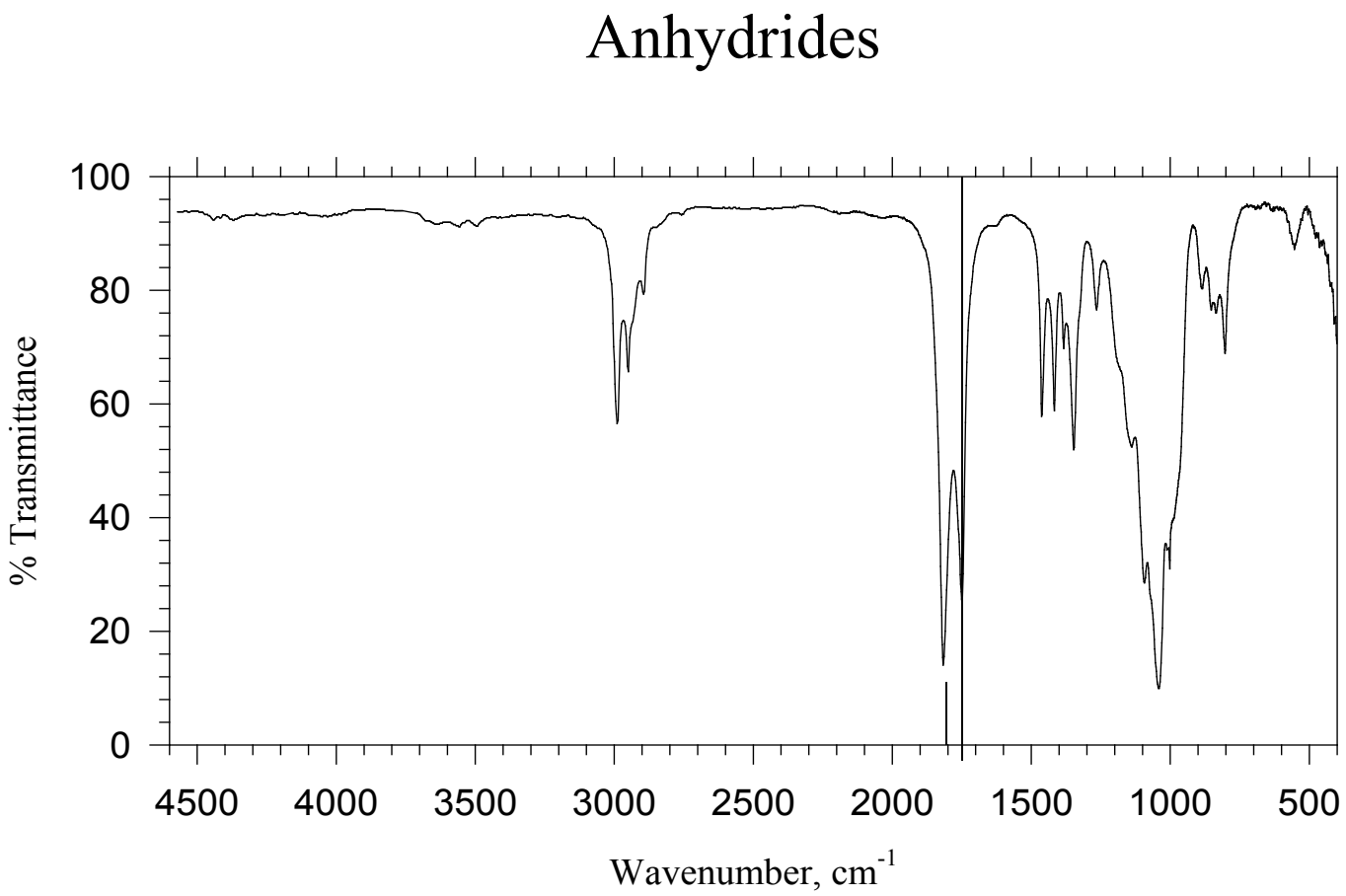


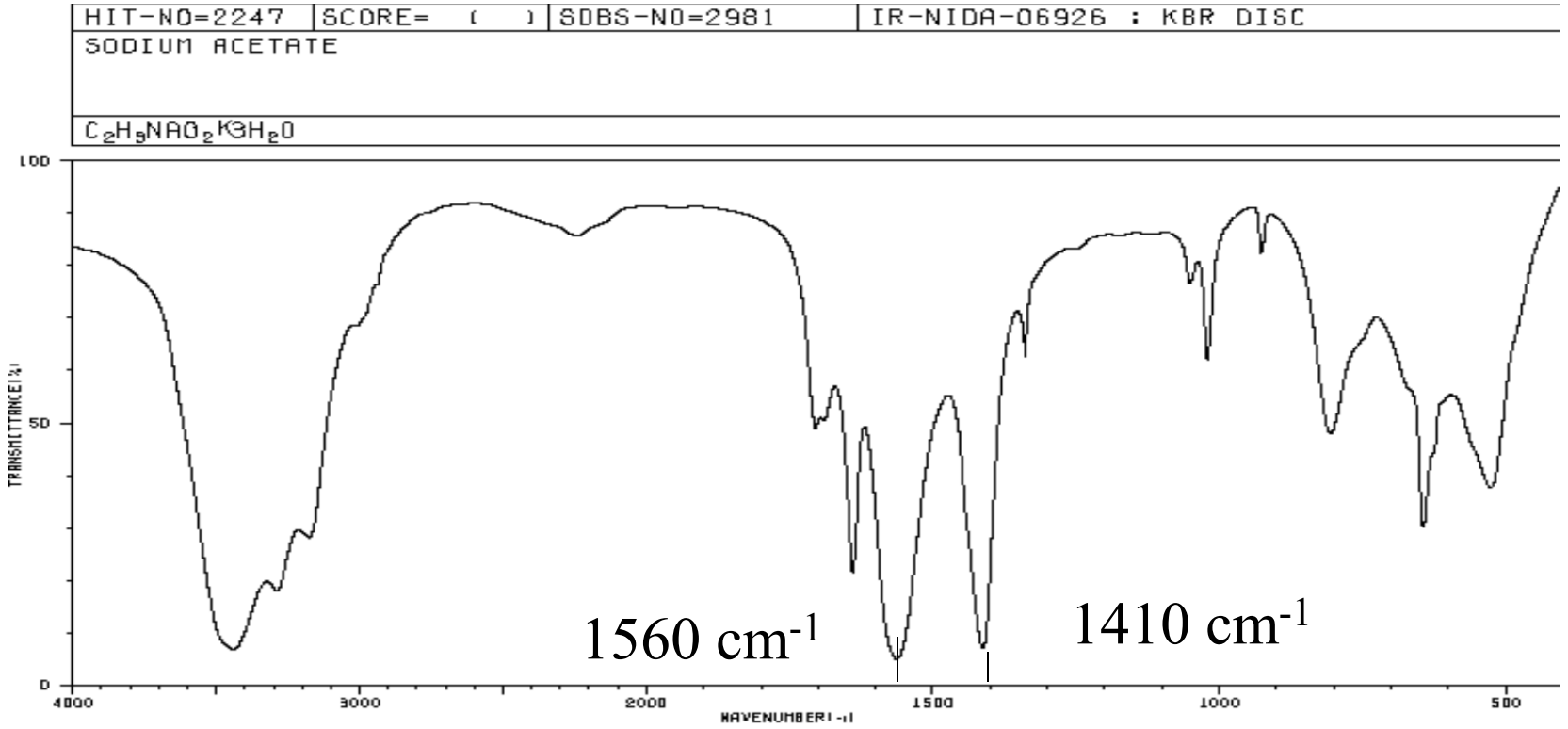
Figure IR-36. Propionic anhydride, neat liquid: $CH_3CH_2CO_2COCH_2CH_3$

The C=O stretching frequency

carboxylates

A summary of the principle infrared bands and their assignments. R is an aliphatic group.

C=O	aldehydes	R(C=O)H	1740-1720	S(sh)	14
	ketones	R(C=O)R	1730-1710	S(sh)	35
	esters	$R(CO_2)R$	1750-1735	S(sh)	33, 34
	carboxylic acids	RCO_2H	1720-1680	S(sh)	26,27,30
	amides (Amide I)	$RCONH_2$, RCONHR	1670-1640	S(sh)	19, 21
	(Amide II)	$RCONH_2$	1650-1620	S(sh)	19, 21
	(Amide II)	RCONHR	1550	S(sh)	19, 21
	amide	$RCONR_2$	1650-1620	S(sh)	23
	anhydrides	$R(CO_2CO)R$	1820, 1750	S, S(sh)	36
	carboxylates	$R(CO_2)^-$, M^+	1600, 1400	S,S(sh)	42

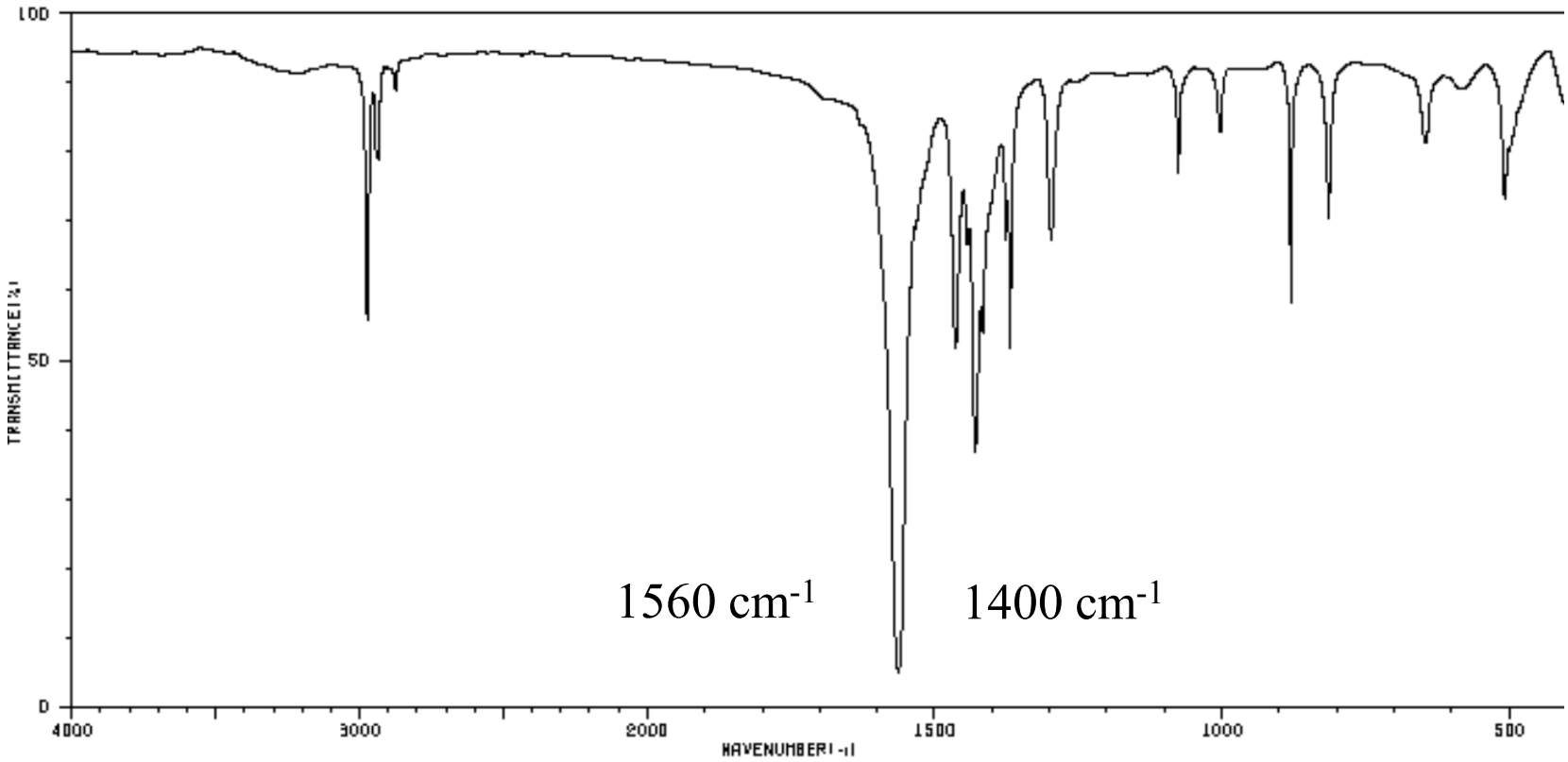


3438	6	1690	49	928	79
3287	17	1640	20	806	46
3176	26	1563	4	645	29
2252	81	1413	6	626	36
2242	81	1339	60		
1705	47	1051	74		
1696	49	1021	60		

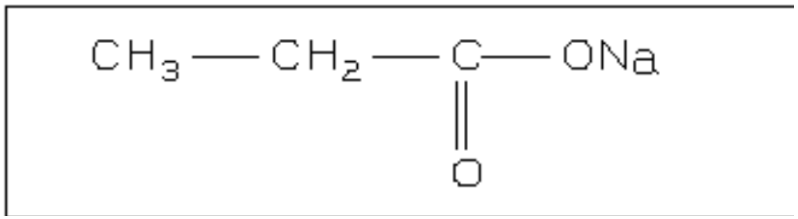
HIT-NO=1057	SCORE= ( )	SDBS-NO=610	IR-NIDA-65698 : KBR DISC

SODIUM PROPIONATE

$C_3H_5NaO_2$



2973	63	1417	62	814	68
2936	77	1377	64	646	79
2874	86	1369	49	640	84
1662	4	1297	64	582	86
1464	49	1076	74	508	70
1443	64	1003	79	503	77
1429	35	880	66		



The C=C bond stretch

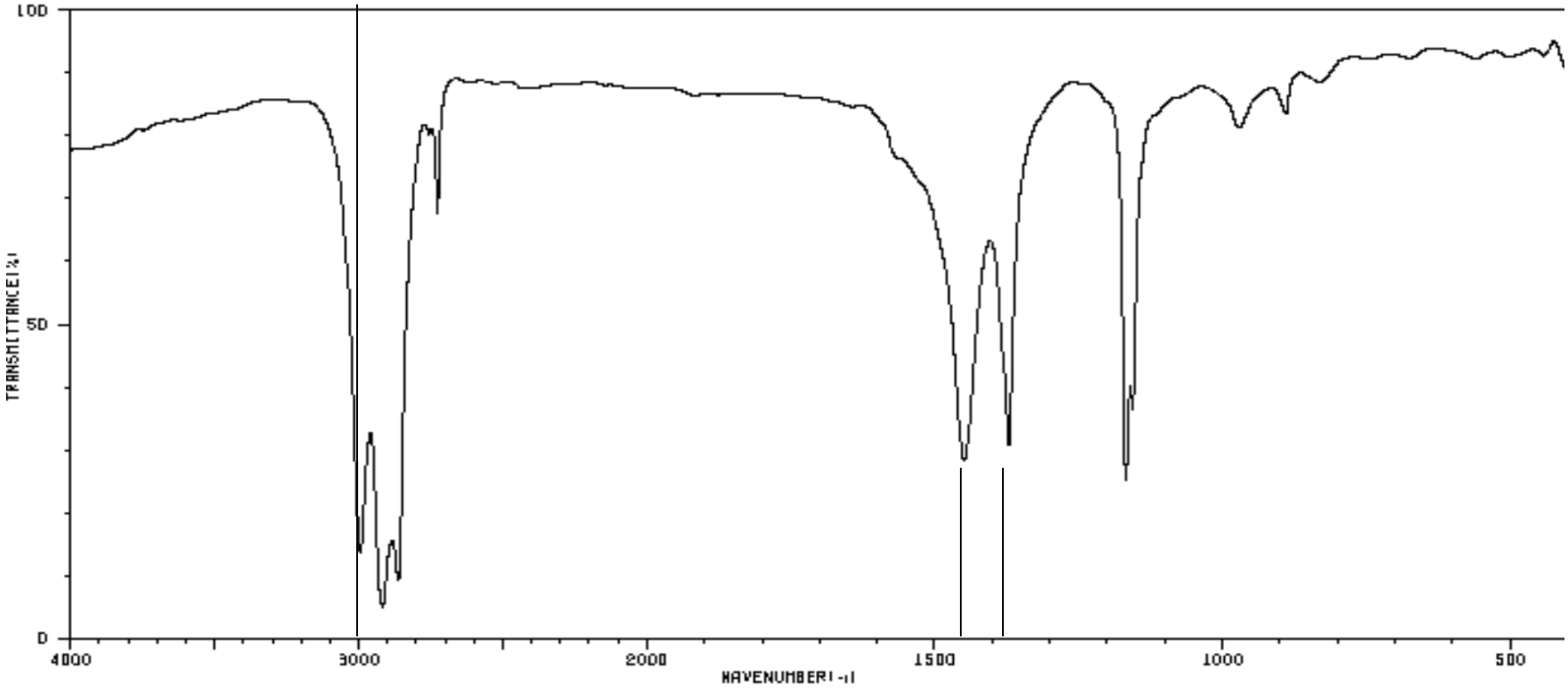
A summary of the principle infrared bands and their assignments. R is an aliphatic group.

C=O	aldehydes	R(C=O)H	1740-1720	S(sh)	14
	ketones	R(C=O)R	1730-1710	S(sh)	35
	esters	$R(CO_2)R$	1750-1735	S(sh)	33, 34
	carboxylic acids	RCO_2H	1720-1680	S(sh)	26,27,30
	amides (Amide I)	$RCONH_2$, RCONHR	1670-1640	S(sh)	19, 21
	(Amide II)	$RCONH_2$	1650-1620	S(sh)	19, 21
	(Amide II)	RCONHR	1550	S(sh)	19, 21
	amide	$RCONR_2$	1650-1620	S(sh)	23
	anhydrides	$R(CO_2CO)R$	1820, 1750	S, S(sh)	36
	carboxylates	$R(CO_2)^-$, M^+	1600, 1400	S,S(sh)	42
C=C	olefins	$R_2C=CR_2$	1680-1640	W(sh)	10, 39, 40
		$R_2C=CH_2$	1600-1675	M(sh)	9, 35
		$R_2C=C(OR)R$	1600-1630	S(sh)	41

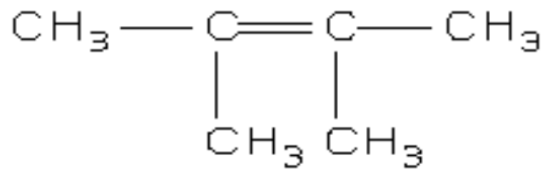
HIT-NO=2802	SCORE= ( )	SDBS-NO=4816	IR-NIDA-03378 : LIQUID FILM

2,3-DIMETHYL-2-BUTENE

C_6H_{12}



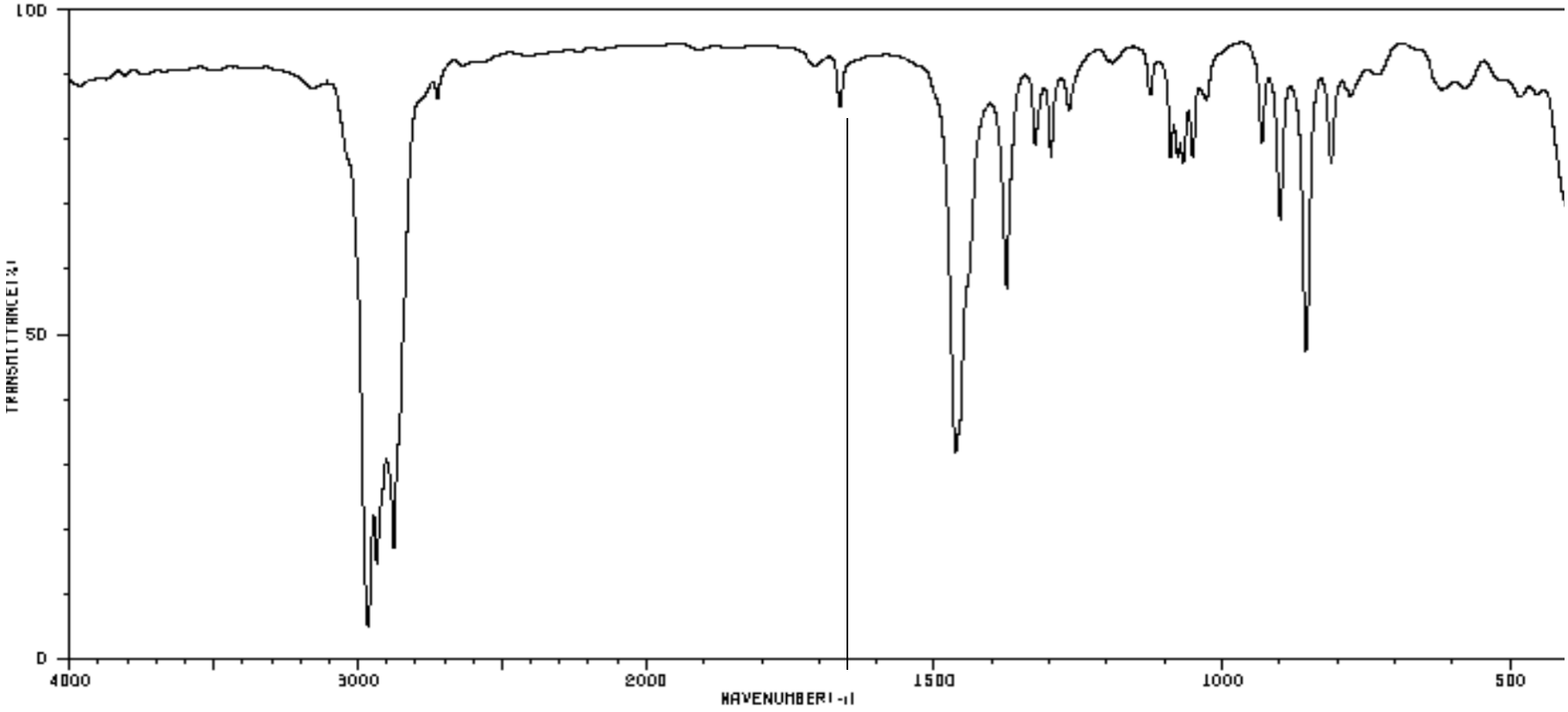
2994	13	1167	36
2918	4	972	79
2863	6	900	61
2726	66	890	79
1449	26	836	84
1371	29	831	84
1169	23		



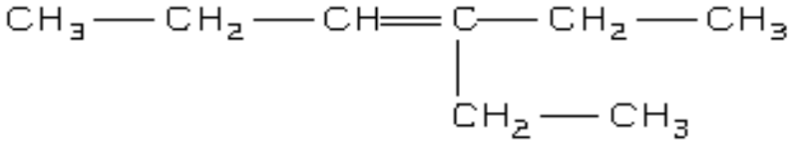
HIT-NO=877	SCORE= ( )	SDBS-NO=191	IR-NIDA-32827 : LIQUID FILM

3-ETHYL-3-HEXENE

C_8H_{16}



3162	84	1374	66	1078	74	811	74
2965	4	1325	77	1067	74	779	84
2935	13	1309	84	1051	74	619	84
2876	16	1298	74	1028	84	578	84
2723	84	1267	81	931	77	482	84
1864	81	1125	84	899	84		
1463	30	1090	74	866	46		



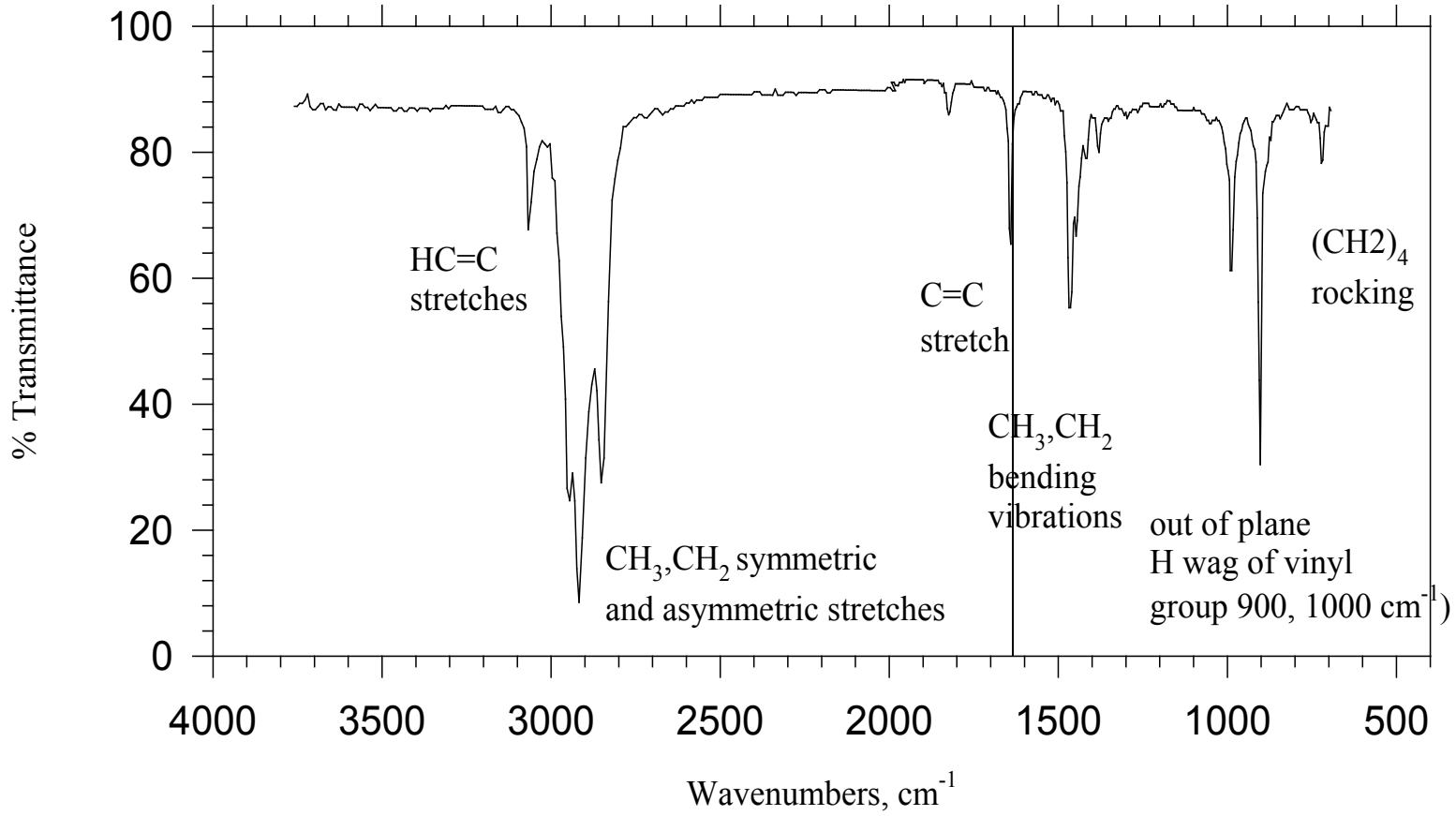


Figure IR-9. 1-Heptene; neat sample, thin film:

$H_2C=CH\text{-}CH_2CH_2CH_2CH_2CH_3$

The C=C bond stretch when next to a heteroatom

A summary of the principle infrared bands and their assignments. R is an aliphatic group.

C=O	aldehydes	R(C=O)H	1740-1720	S(sh)	14
	ketones	R(C=O)R	1730-1710	S(sh)	35
	esters	$R(CO_2)R$	1750-1735	S(sh)	33, 34
	carboxylic acids	RCO_2H	1720-1680	S(sh)	26,27,30
	amides (Amide I)	$RCONH_2$, RCONHR	1670-1640	S(sh)	19, 21
	(Amide II)	$RCONH_2$	1650-1620	S(sh)	19, 21
	(Amide II)	RCONHR	1550	S(sh)	19, 21
	amide	$RCONR_2$	1650-1620	S(sh)	23
	anhydrides	$R(CO_2CO)R$	1820, 1750	S, S(sh)	36
	carboxylates	$R(CO_2)^-$, M^+	1600, 1400	S,S(sh)	42
C=C	olefins	$R_2C=CR_2$	1680-1640	W(sh)	10, 39, 40
		$R_2C=CH_2$	1600-1675	M(sh)	9, 35
		$R_2C=C(OR)R$	1600-1630	S(sh)	41

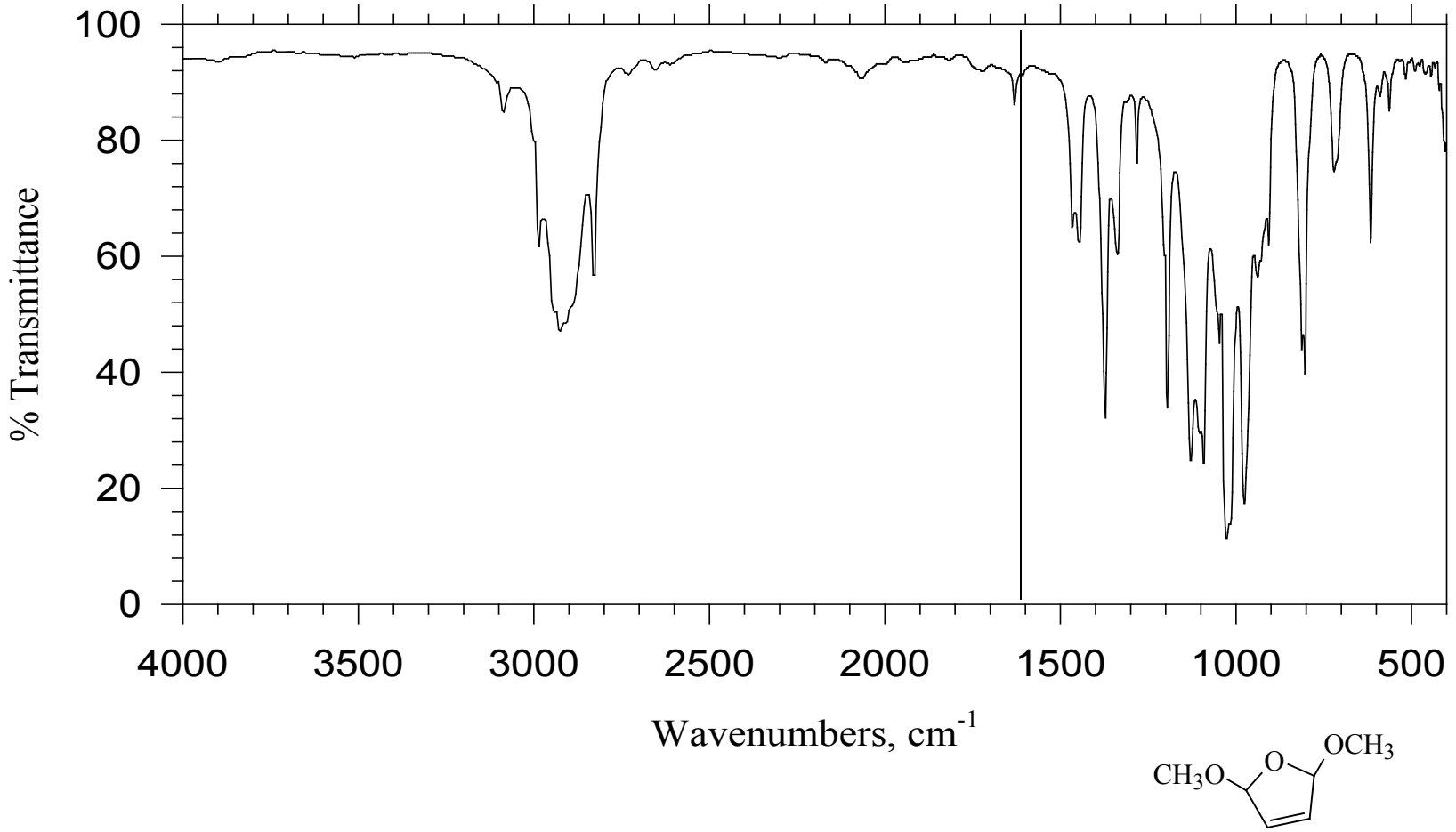


Figure IR-40. 2,5-Dimethoxy2,5-dihydrofuran, neat liquid:

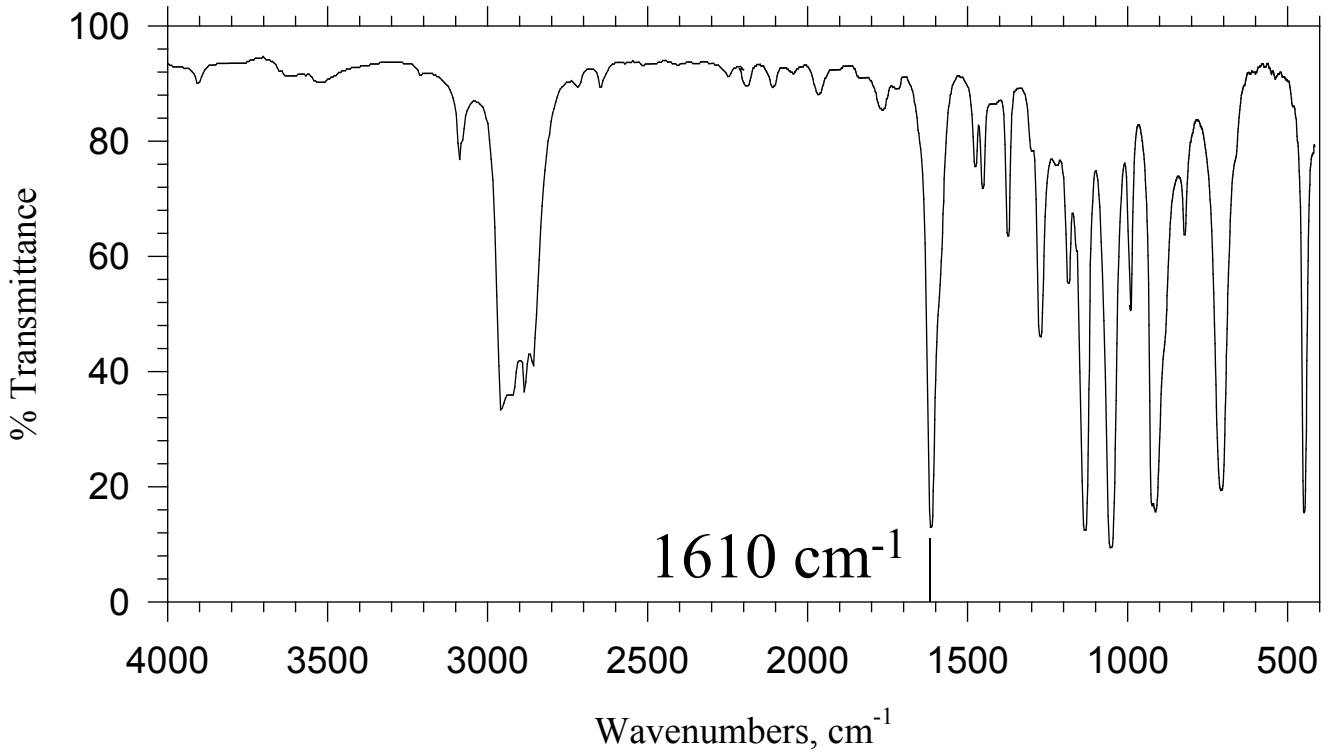
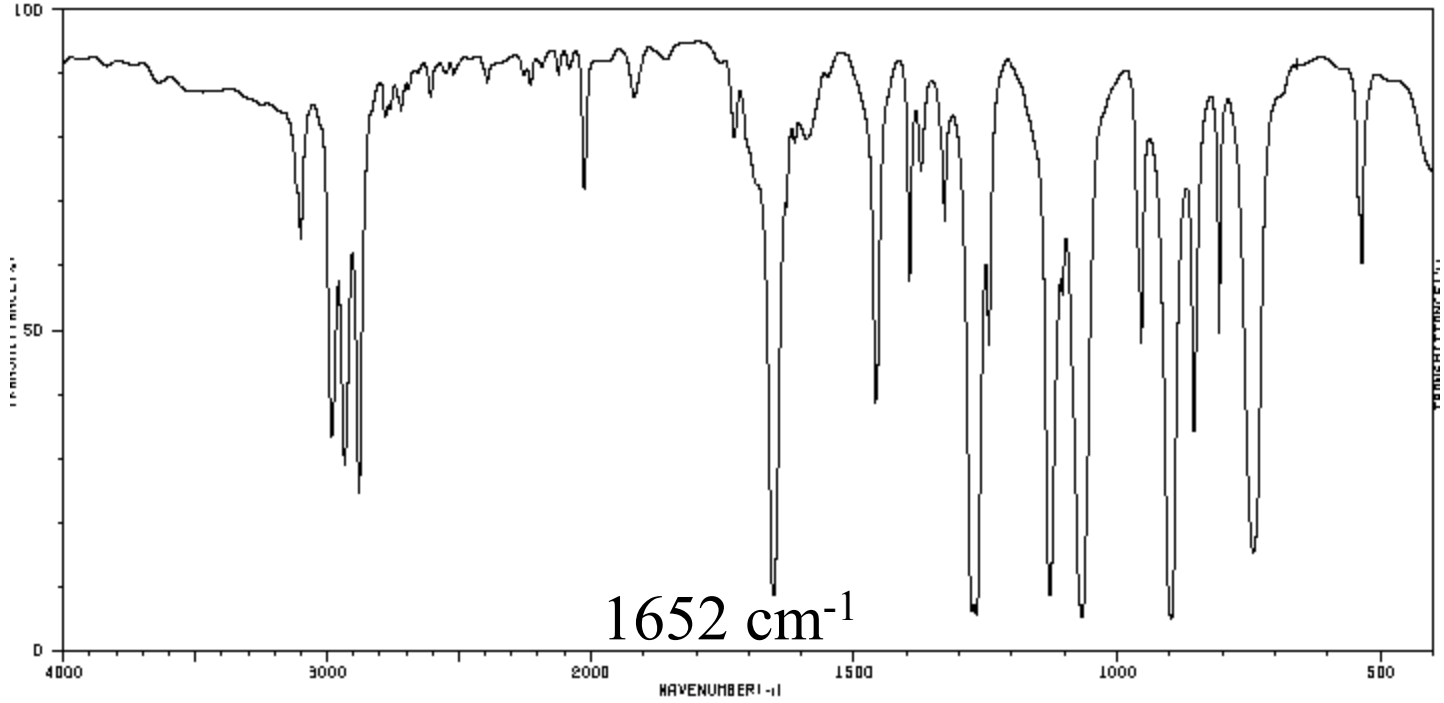


Figure IR-41. 2,3-Dihydrofuran, neat liquid:

HIT-NO=449	SCORE= ( )	SDBS-NO=35998	IR-NIDA-56870 : LIQUID FILM

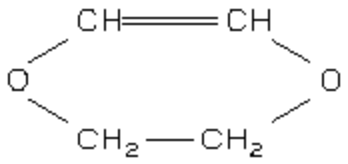
2,3-DIHYDRO-1,4-DIOXIN

$C_4H_6O_2$



1652 cm^{-1}

3129	77	2760	81	1917	84	1373	72	1067	5
3100	62	2719	81	1728	77	1328	64	955	46
2982	32	2690	84	1652	6	1276	5	898	4
2963	62	2607	84	1613	77	1268	5	864	33
2934	28	2522	86	1590	77	1244	46	807	47
2879	23	2228	84	1459	37	1128	8	742	14
2779	79	2024	70	1396	66	1104	53	636	58

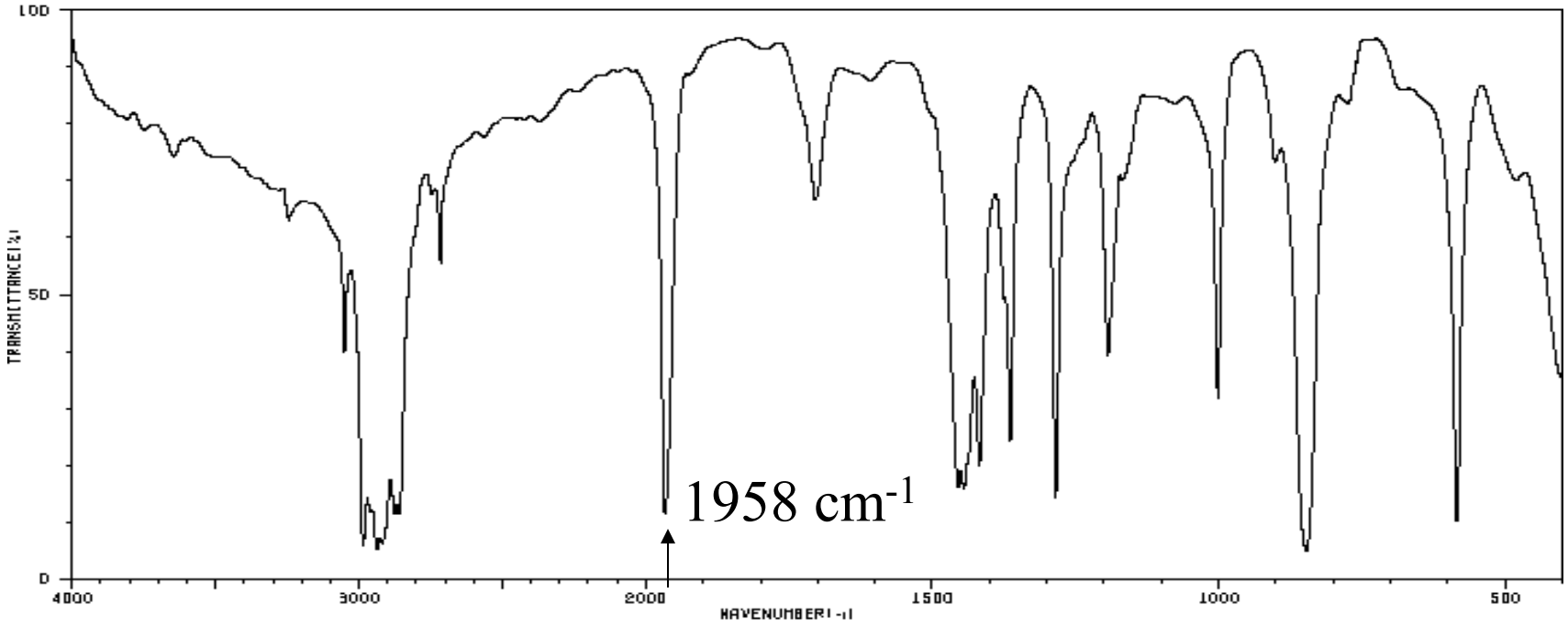


The cumulative C=C bond stretch

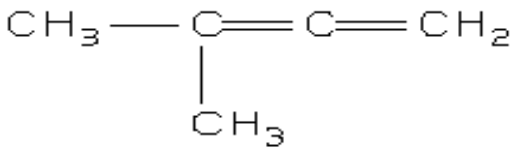
HIT-NO=2941	SCORE= ( )	SDBS-NO=5384	IR-NIDA-13611 : LIQUID FILM

3-METHYL-1.2-BUTADIENE

C_5H_8



3749	77	2876	10	1607	84	1194	37
3646	72	2860	10	1455	15	1002	30
3246	80	2747	64	1445	15	901	70
3061	38	2716	69	1418	19	847	4
2984	5	2563	74	1375	47	776	79
2936	5	1968	10	1364	23	585	9
2918	6	1704	64	1286	13	481	68



The NO_2 stretching frequency

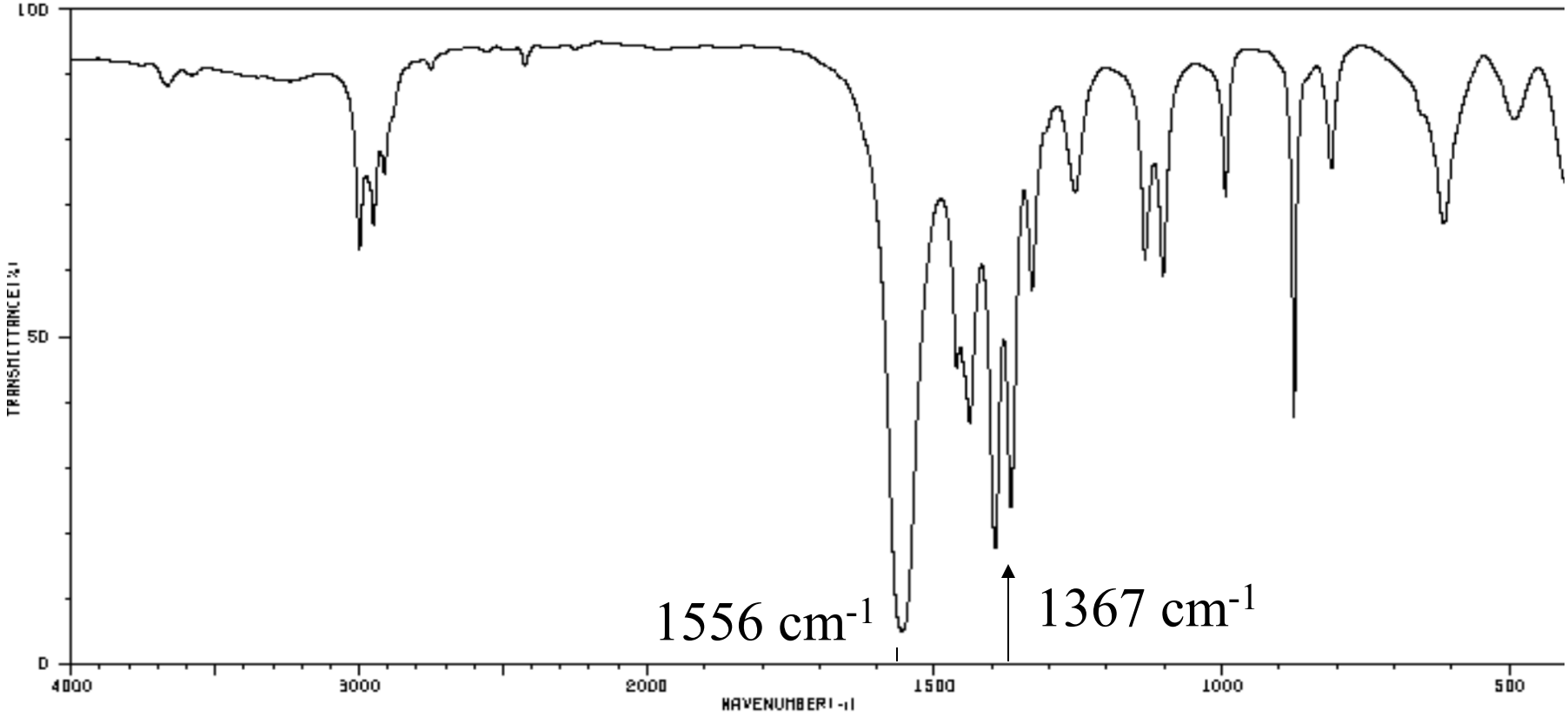
A summary of the principle infrared bands and their assignments. R is an aliphatic group.

C=O	aldehydes	R(C=O)H	1740-1720	S(sh)	14
	ketones	R(C=O)R	1730-1710	S(sh)	35
	esters	$R(CO_2)R$	1750-1735	S(sh)	33, 34
	carboxylic acids	RCO_2H	1720-1680	S(sh)	26,27,30
	amides (Amide I)	$RCONH_2$, RCONHR	1670-1640	S(sh)	19, 21
	(Amide II)	$RCONH_2$	1650-1620	S(sh)	19, 21
	(Amide II)	RCONHR	1550	S(sh)	19, 21
	amide	$RCONR_2$	1650-1620	S(sh)	23
	anhydrides	$R(CO_2CO)R$	1820, 1750	S, S(sh)	36
	carboxylates	$R(CO_2)^-$, M^+	1600, 1400	S,S(sh)	42
C=C	olefins	$R_2C=CR_2$	1680-1640	W(sh)	10, 39, 40
		$R_2C=CH_2$	1600-1675	M(sh)	9, 35
		$R_2C=C(OR)R$	1600-1630	S(sh)	41
$-NO_2$	nitro groups	RNO_2	1550, 1370	S,S(sh)	28

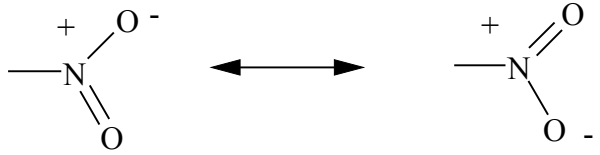
HIT-NO=953	SCORE= ( )	SDBS-NO=309	IR-NIDA-67212 : LIQUID FILM

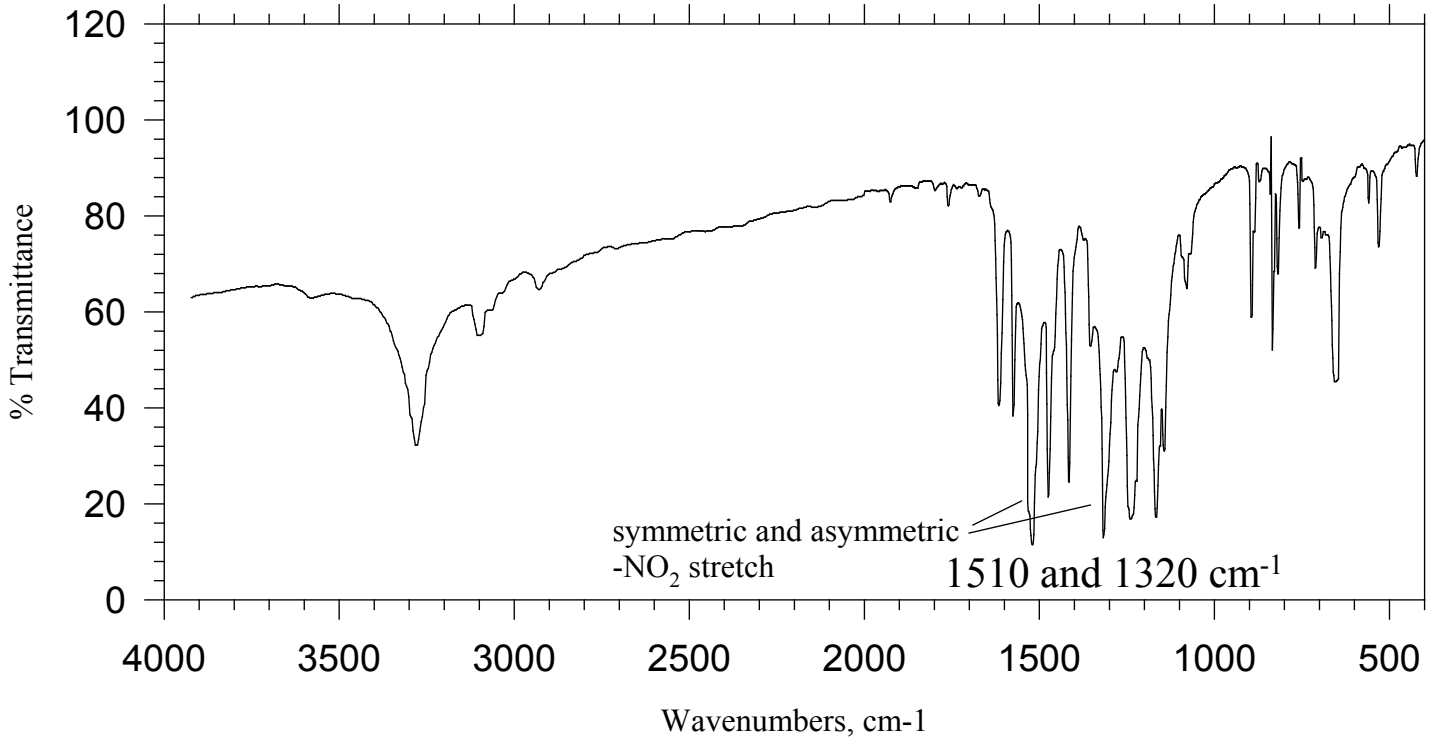
NITROETHANE

$C_2H_5NO_2$



3667	84	1396	17	876	36
2999	60	1367	23	810	72
2950	84	1331	55	815	84
2912	72	1266	70	491	79
1556	4	1134	58		
1462	43	1102	57		
1439	36	994	68		





4-Chloro-2-nitrophenol, KBr pellet:

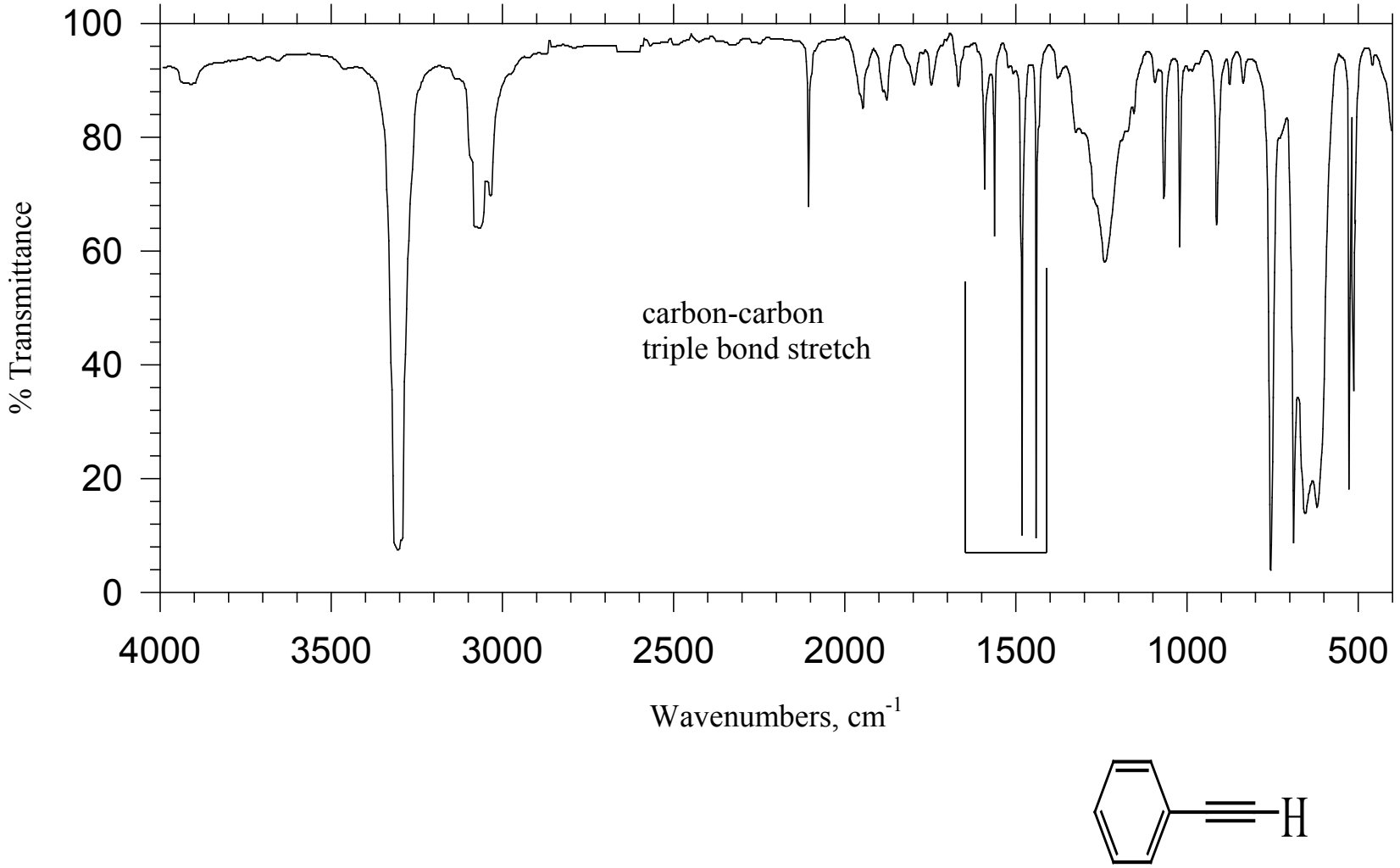
Aromatic Rings

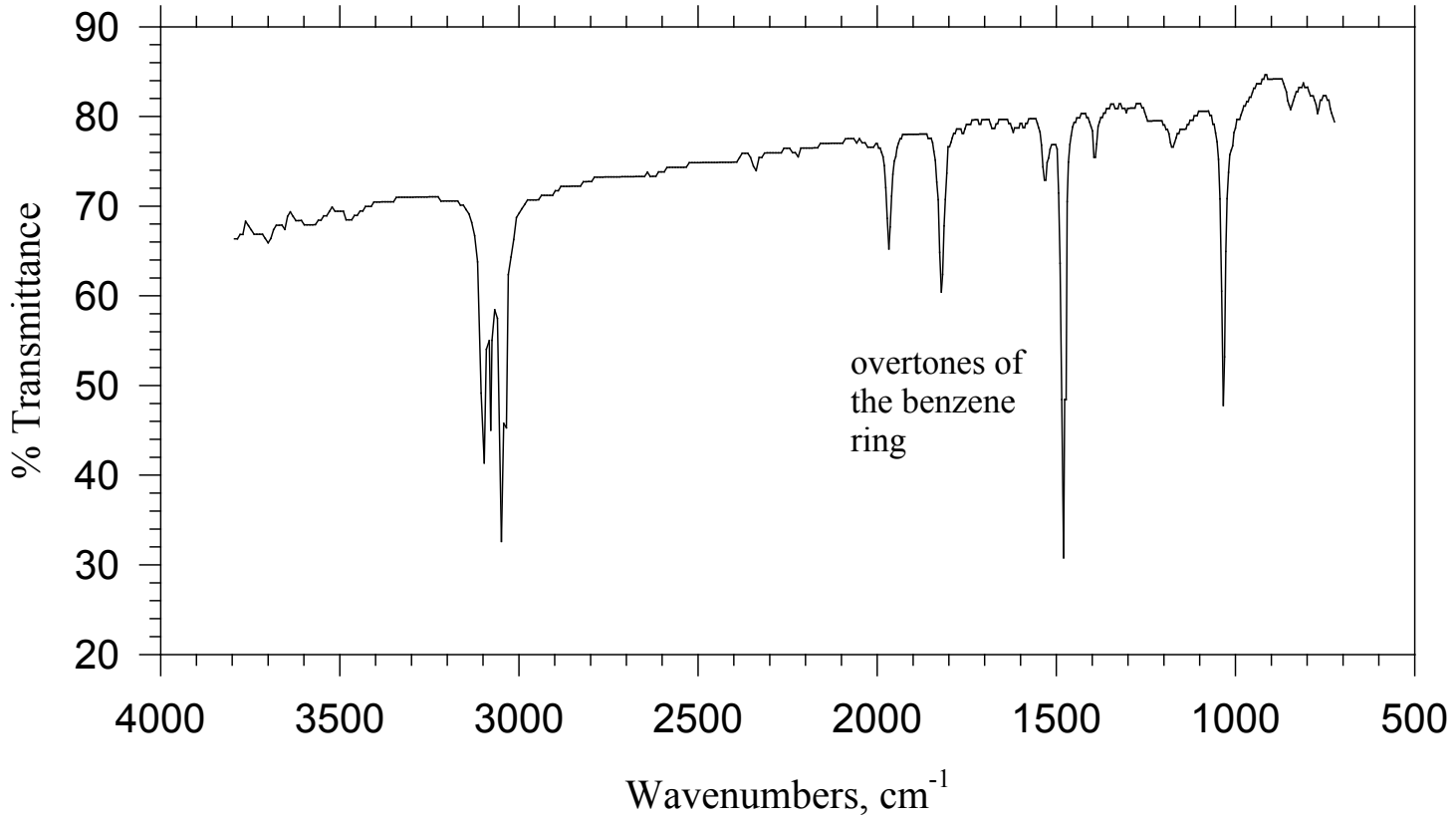
Ring breathing motions

1600-1585

1500-1400

Both often appear as doublets


100
80
60
40
20
0
% Transmittance
4000
3500
3000
2500
2000
1500
1000
500
Wavenumbers, cm-1
carbon-carbon
triple bond stretch
H



Benzene, neat, thin film: