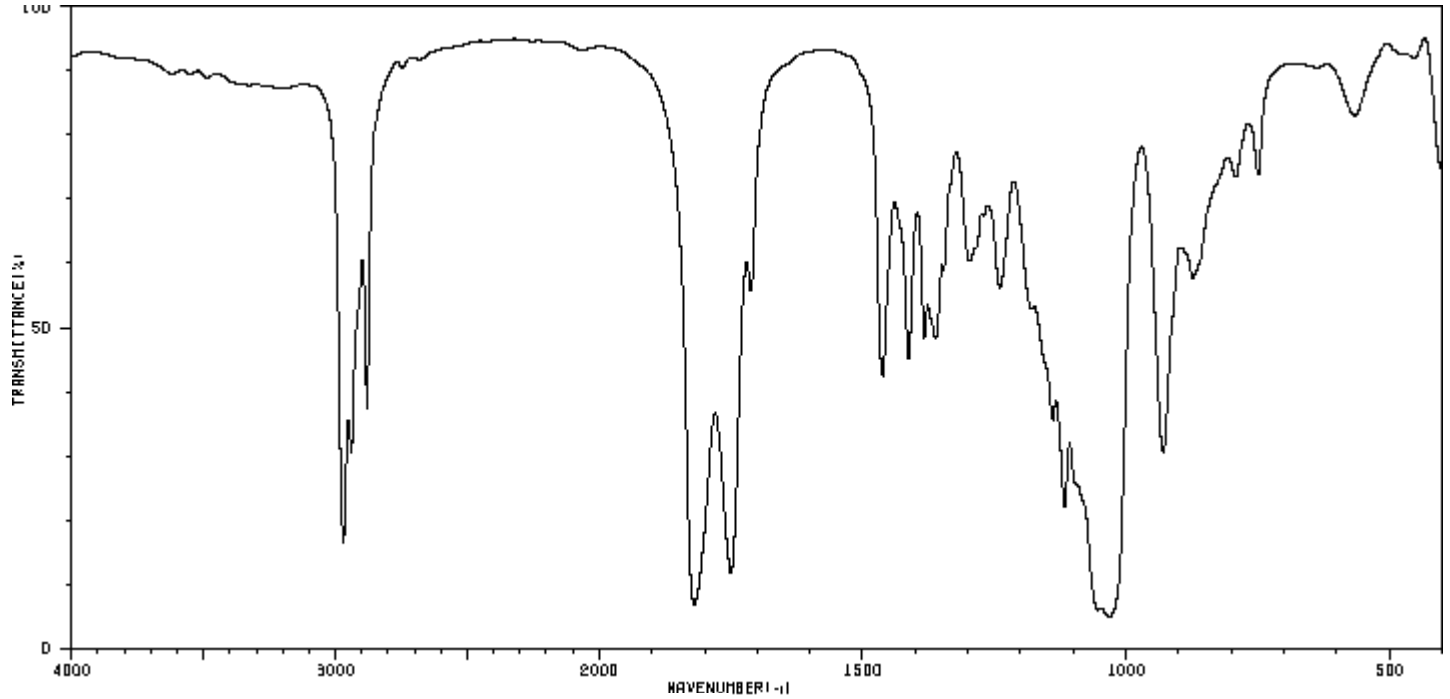
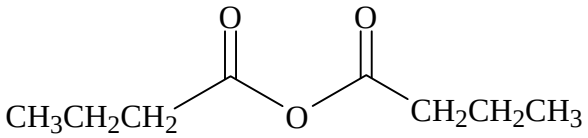
Using IR to Solve Problems

Match the infrared spectrum given below with one of the following compounds:



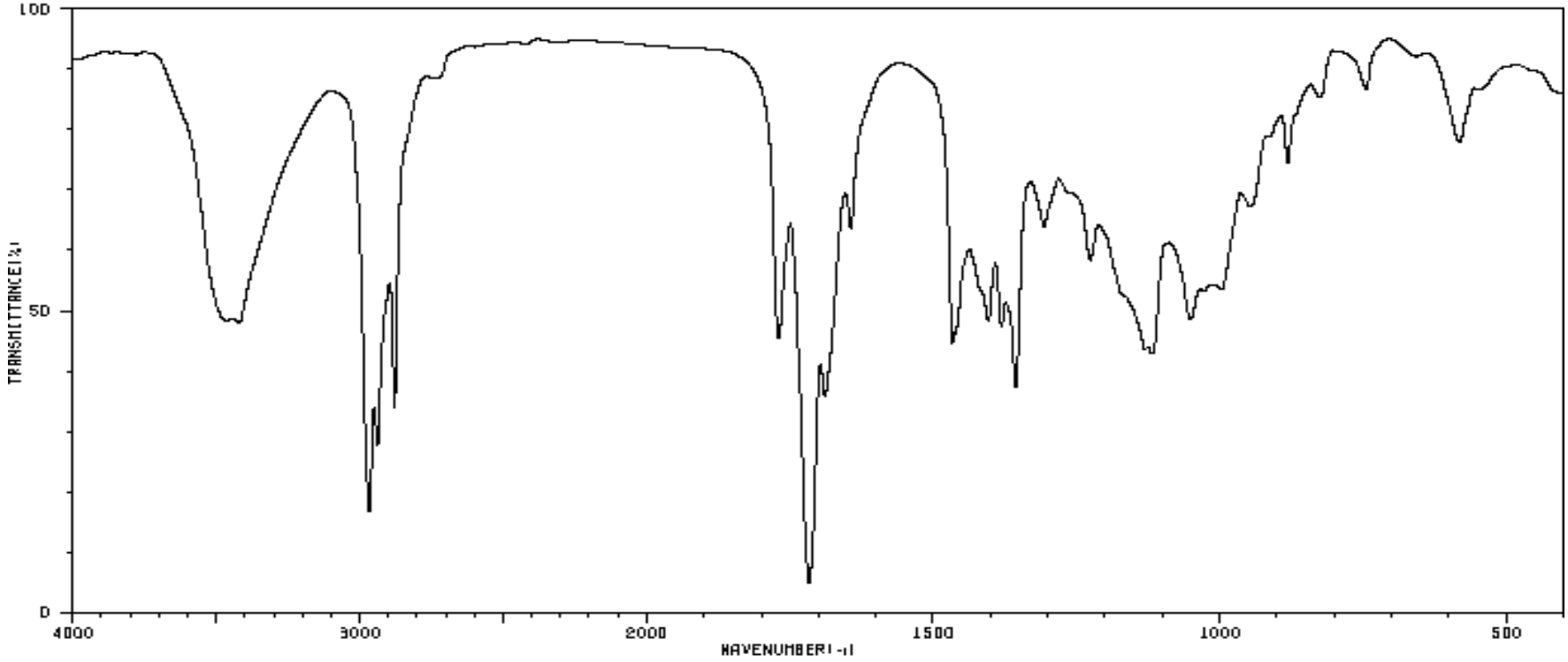
2970	16	1413	43	1116	21	666	79
2940	29	1383	46	1039	5		
2880	36	1362	46	1031	4		
1819	6	1297	68	929	29		
1750	11	1287	60	874	55		
1712	53	1240	59	792	70		
1461	41	1140	34	749	70		



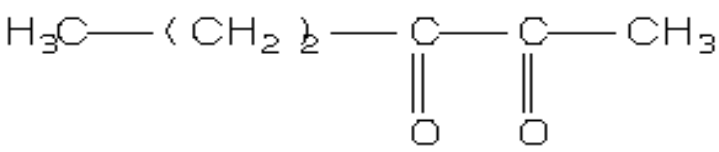
HIT-NO=3979	SCORE= ( )	SDBS-NO=10104	IR-NIDA-02277 : LIQUID FILM

2,3-HEXANEDIONE

$C_6H_{10}O_2$



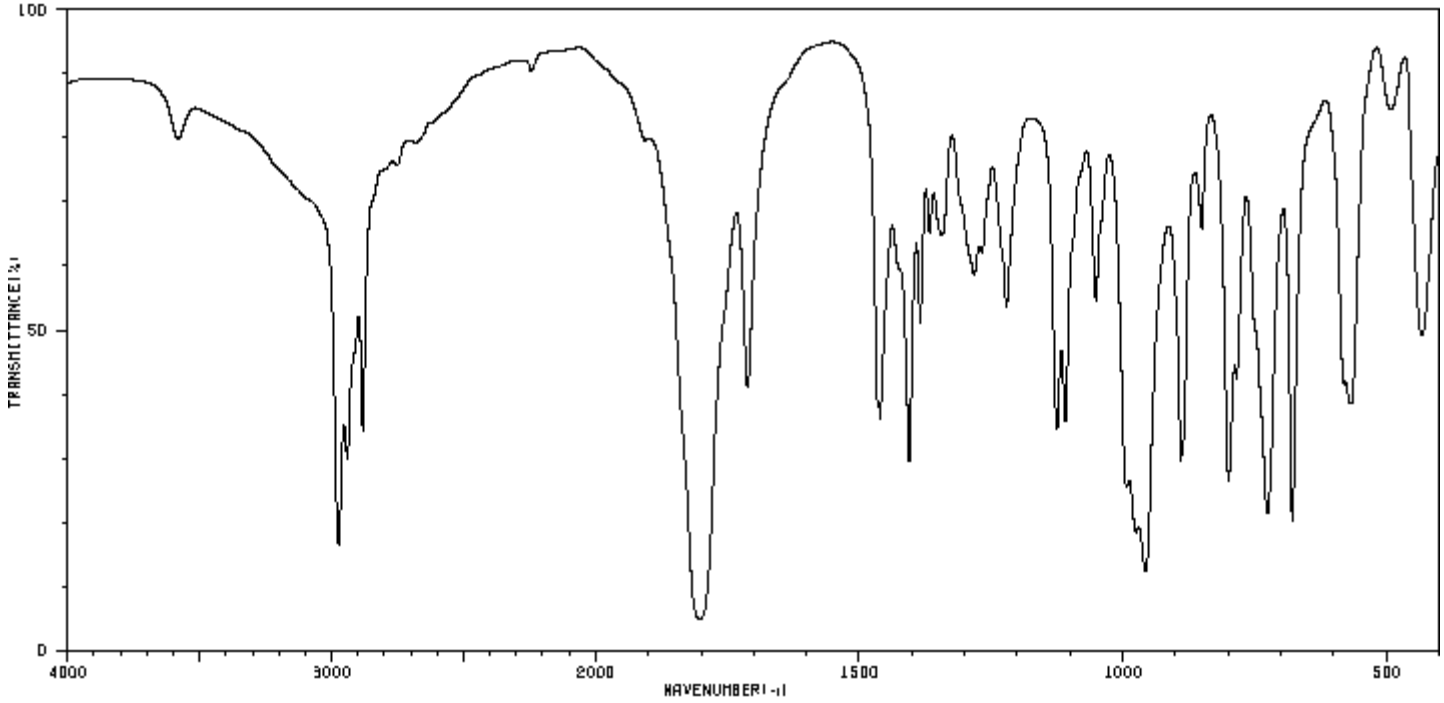
3449	46	1644	60	1227	67	824	81
2967	16	1467	42	1130	42	755	86
2938	26	1461	44	1125	42	745	84
2878	32	1404	46	1118	41	582	74
1770	43	1381	46	1051	46		
1717	4	1358	56	946	84		
1689	34	1307	62	882	72		



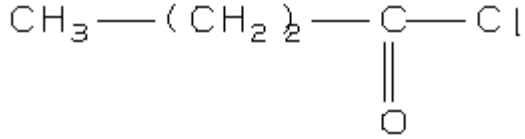
HIT-NO=2578	SCORE= ( )	SDBS-NO=4243	IR-NIDA-01958 : LIQUID FILM

BUTYRYL CHLORIDE

C_4H_7ClO



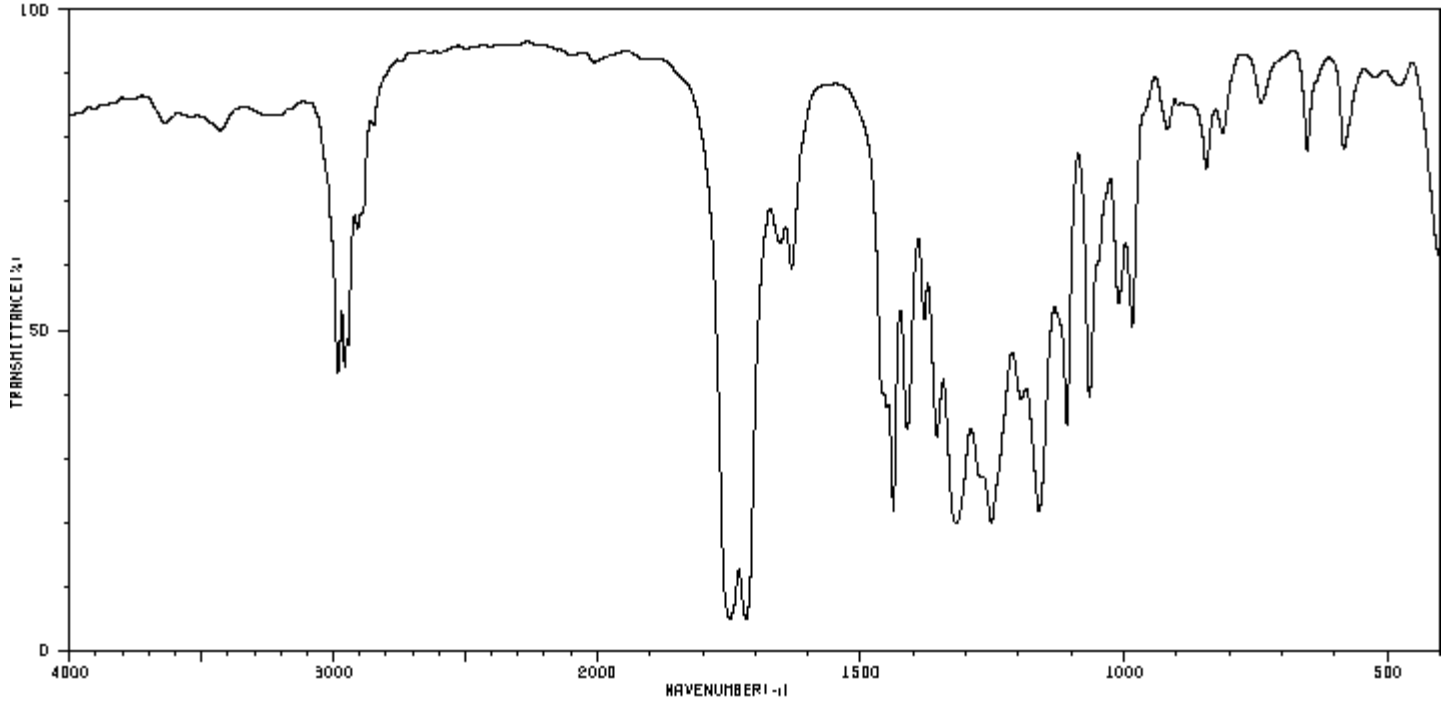
3681	77	1460	34	1126	33	800	26	492	61
2973	16	1406	28	1109	34	784	41	434	47
2941	26	1384	49	1051	52	726	20		
2882	33	1367	62	976	17	679	19		
1802	4	1344	62	957	12	581	39		
1712	39	1283	57	890	26	574	38		
1465	37	1221	52	860	64	568	37		



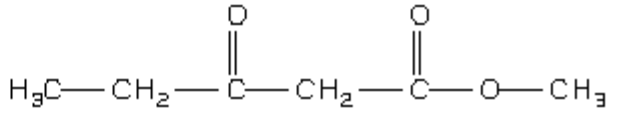
HIT-NO=5727	SCORE= ( )	SDBS-NO=19476	IR-NIDA-68538 : LIQUID FILM

METHYL 3-OXOVALERATE

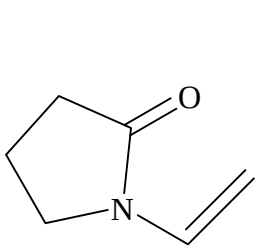
$C_6H_{10}O_3$

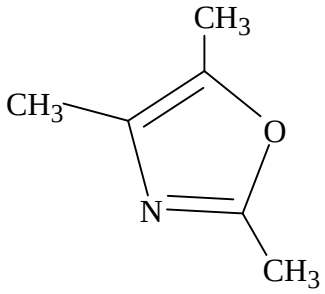


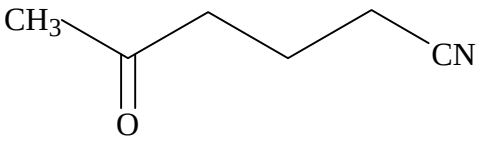
3640	79	1718	4	1366	32	1010	62	663	74
3429	79	1653	60	1319	19	985	49	583	74
2982	42	1631	57	1252	19	917	79	478	64
2957	42	1461	36	1196	37	911	81		
2944	46	1438	21	1161	21	844	72		
2910	64	1412	39	1109	34	813	77		
1748	4	1380	60	1066	38	740	81		

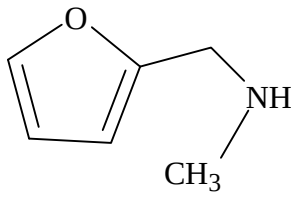


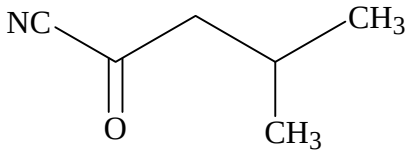
Infrared spectra for the following compounds are shown below. Assign structures to each spectrum and justify your assignment.

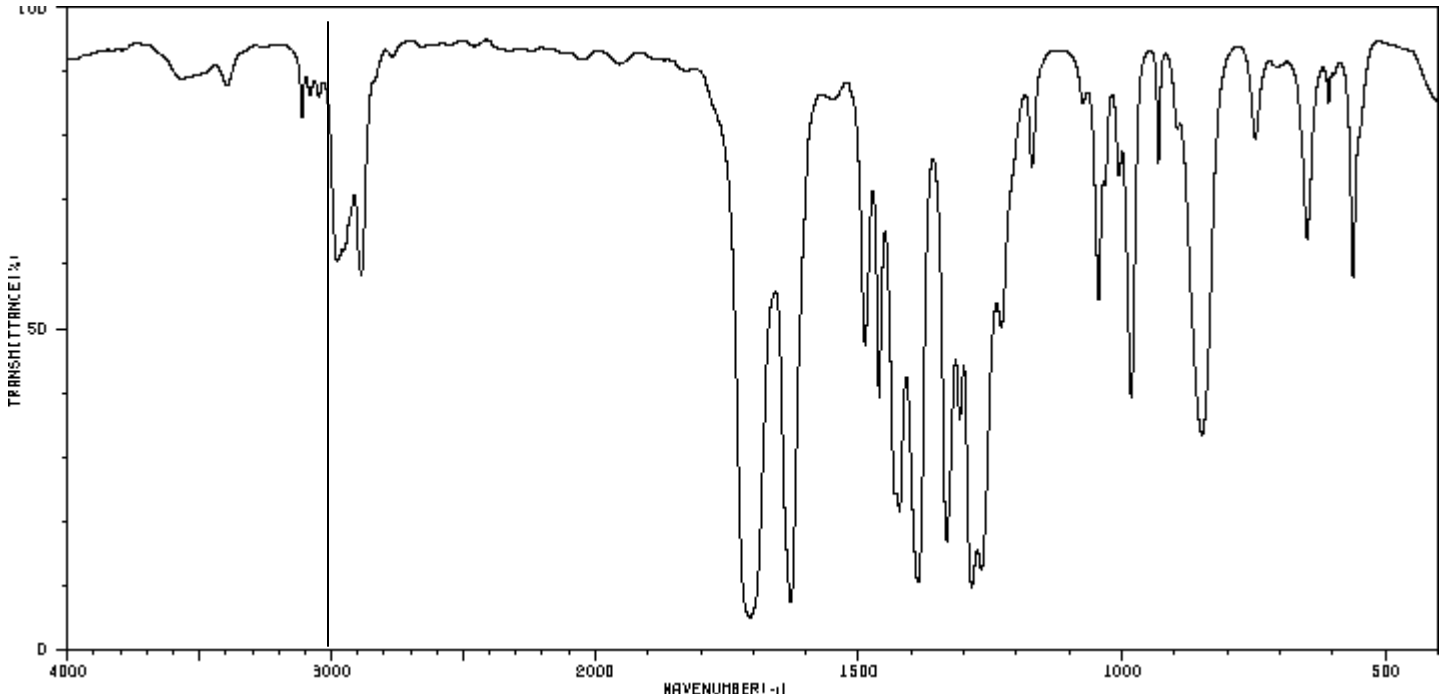




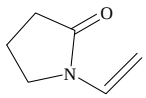


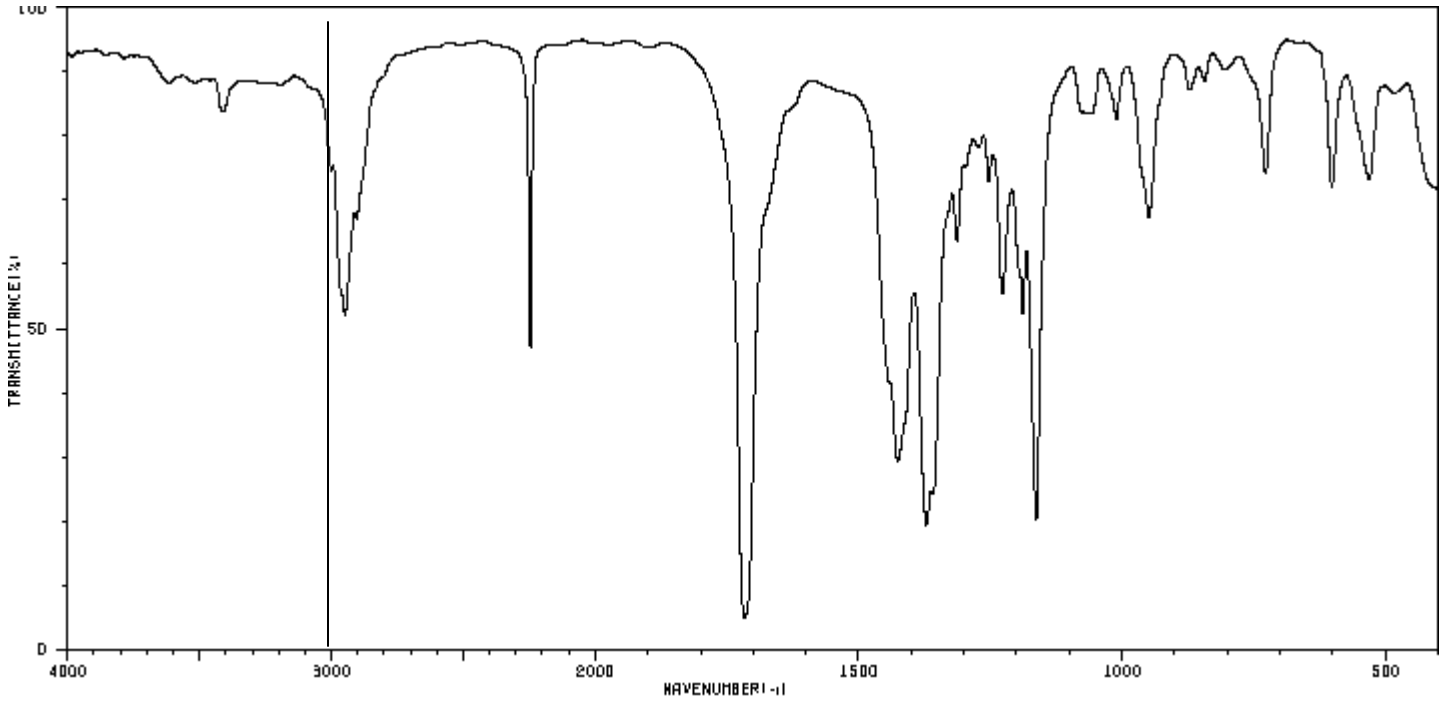




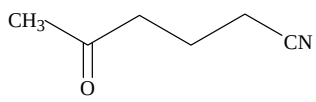


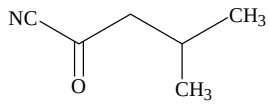
3396	84	2887	67	1388	10	1076	81	747	77
3111	79	1706	4	1333	16	1045	52	649	62
3081	84	1629	7	1308	34	1033	70	609	61
3046	81	1488	44	1286	9	1006	70	601	86
2977	58	1461	37	1267	12	983	37	582	55
2966	56	1430	29	1230	49	931	72		
2952	60	1423	20	1171	72	848	32		

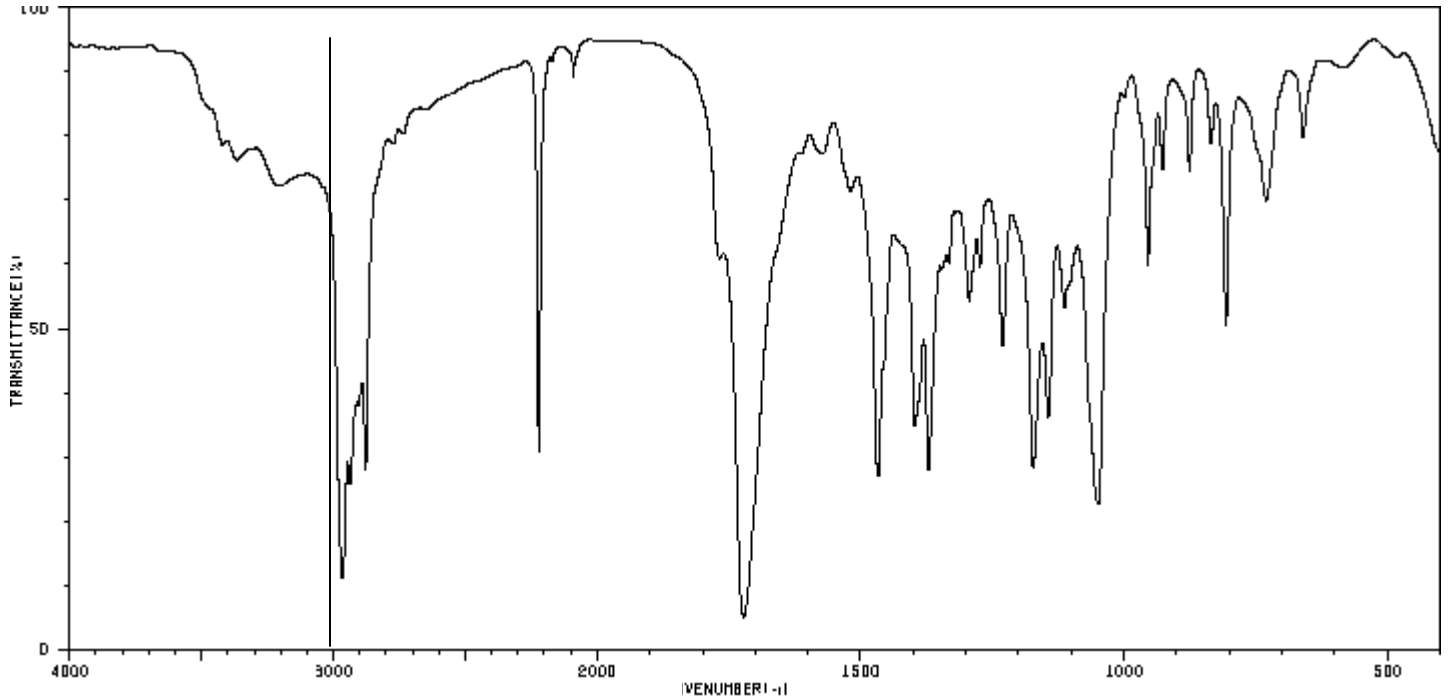




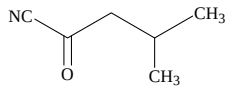
3617	84	1369	29	1164	19	862	86
3411	81	1314	60	1071	81	843	84
2948	50	1273	74	1066	79	728	72
2246	44	1264	70	1061	79	602	70
1716	4	1228	53	1010	79	531	70
1426	28	1198	57	949	84	483	84
1371	18	1189	60	872	84		







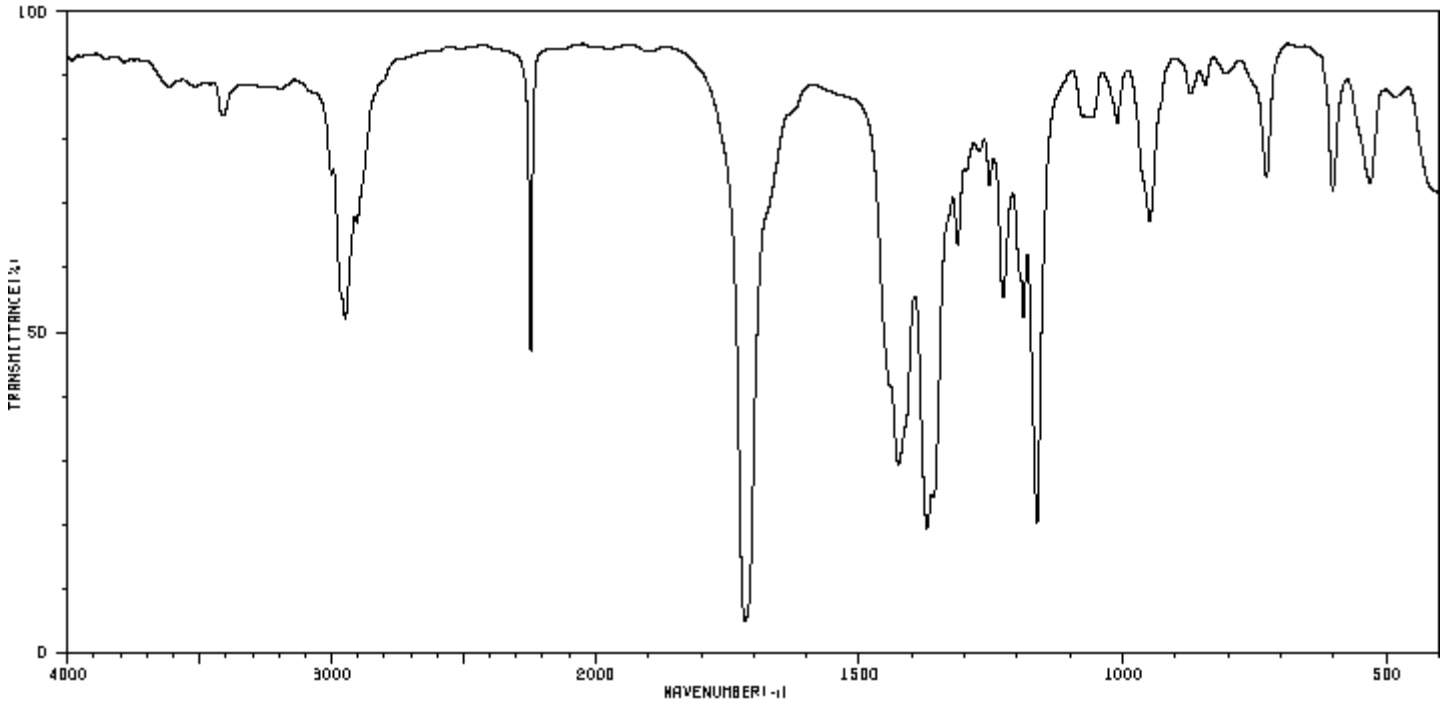
3366	72	2091	86	1333	68	1104	66	731	66
3206	70	1722	4	1294	52	1049	21	661	77
3196	70	1573	74	1274	57	955	57		
2966	10	1519	68	1231	46	927	72		
2935	24	1467	26	1173	26	876	72		
2877	26	1397	33	1144	34	836	77		
2221	29	1371	26	1113	60	807	49		



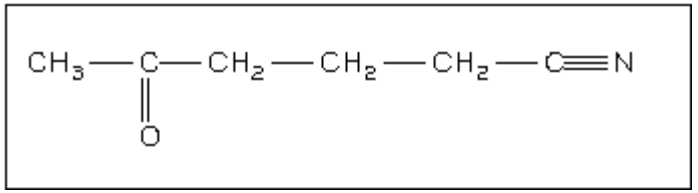
HIT-NO=5452	SCORE= ( )	SDBS-NO=18610	IR-NIDA-37029 : LIQUID FILM

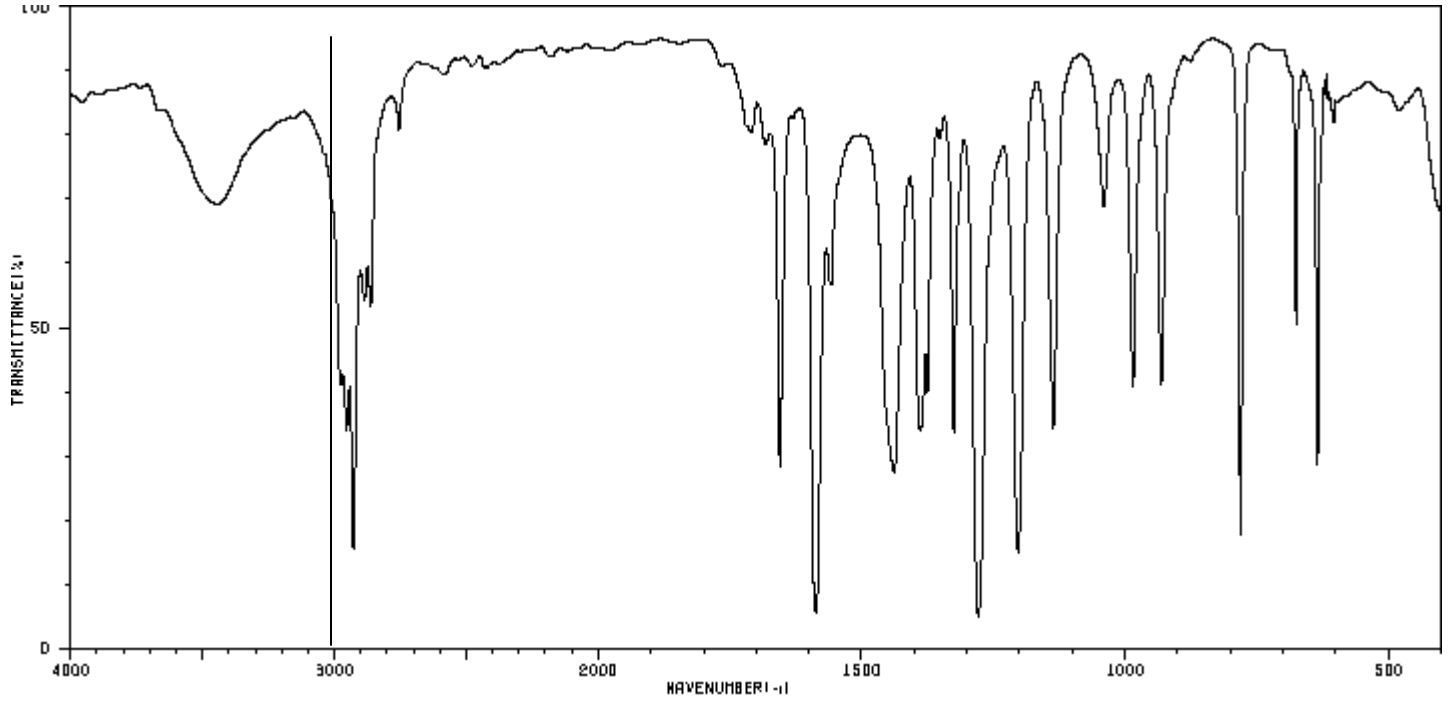
5-OXOHEXANENITRILE

C_6H_9NO

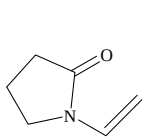


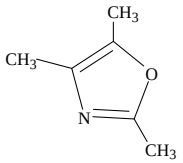
3617	84	1369	29	1164	19	862	86
3411	81	1314	60	1071	81	843	84
2948	50	1273	74	1066	79	728	72
2245	44	1264	70	1061	79	602	70
1716	4	1228	53	1010	79	531	70
1426	26	1198	57	949	84	483	84
1371	18	1189	60	872	84		

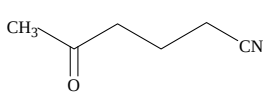


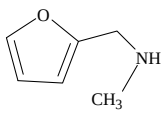


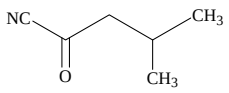
3460	66	2766	77	1668	66	1203	14	636	27
3440	66	2582	86	1439	26	1136	33	625	81
2976	39	1719	79	1390	33	1041	66	615	61
2963	33	1709	77	1376	30	986	30	604	79
2928	14	1683	74	1352	77	931	39	597	81
2886	52	1655	26	1325	32	781	17	591	61
2863	60	1687	6	1279	4	676	40	480	81

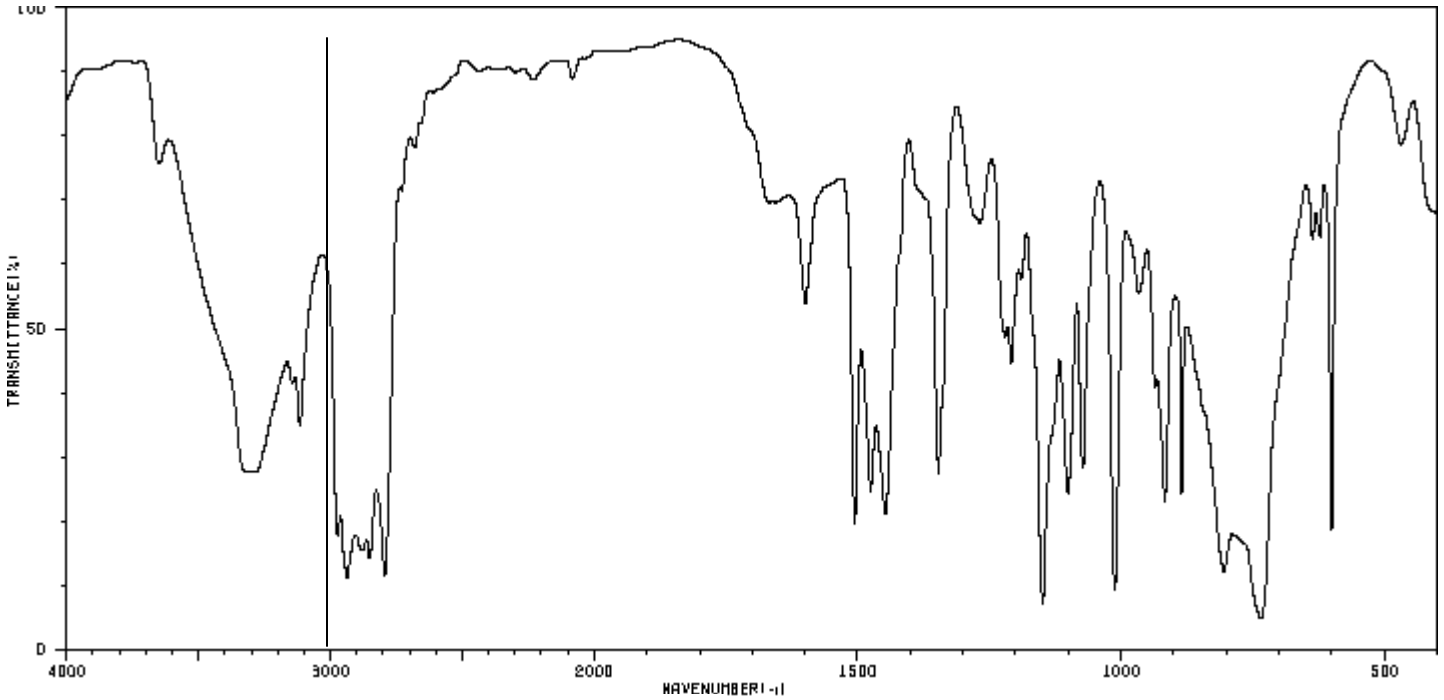




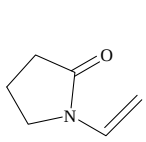


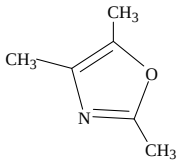


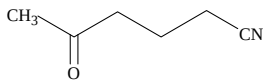


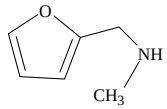


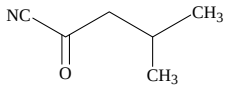
3660	72	2878	16	1447	20	1149	7	686	23
3307	26	2852	13	1347	26	1100	23	806	12
3297	26	2795	11	1279	86	1073	27	735	4
3287	26	2681	74	1268	64	1012	9	637	62
3116	34	1599	52	1220	47	966	53	623	62
2973	17	1505	19	1209	43	935	39	600	18
2936	10	1476	29	1190	66	917	22	468	77







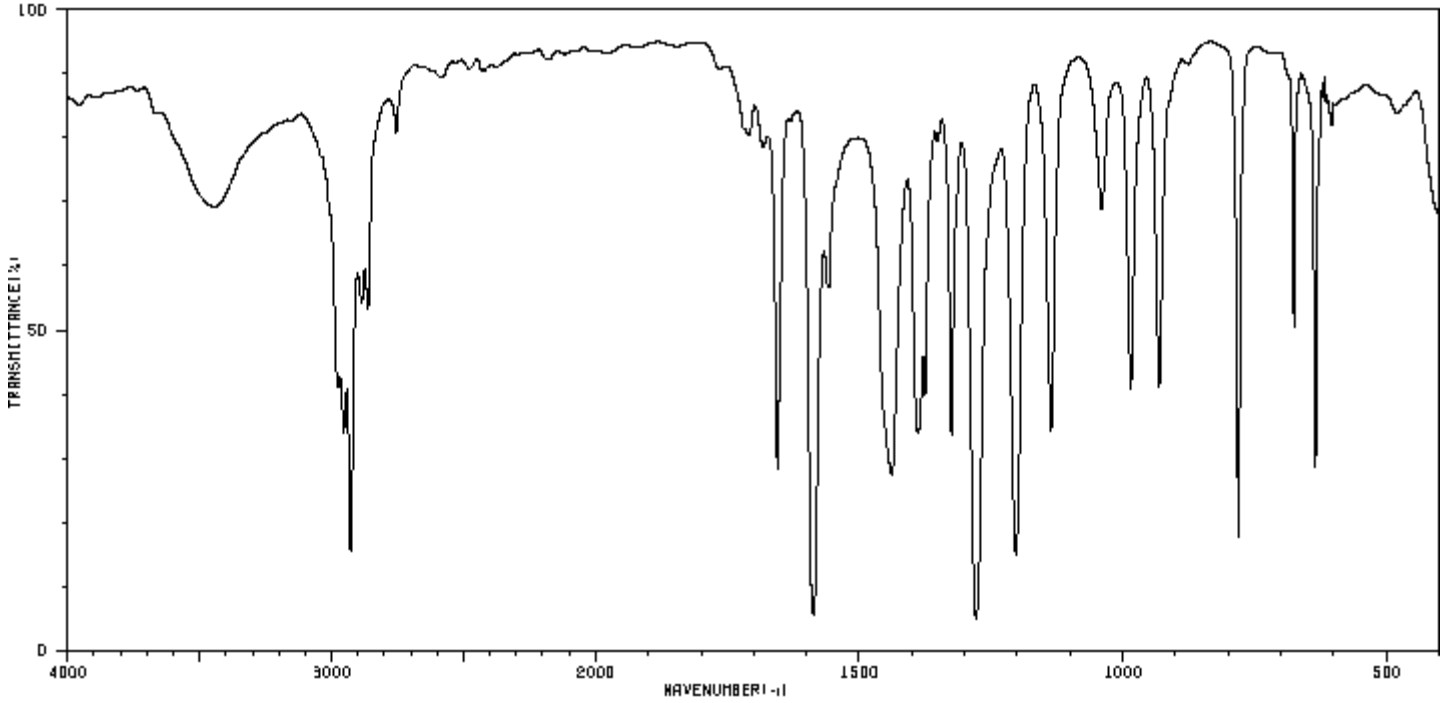




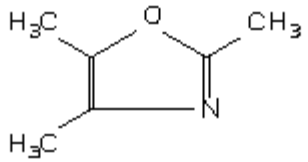
HIT-NO=146	SCORE= ( )	SDBS-NO=23678	IR-NIDA-53188 : LIQUID FILM

2,4,5-TRIMETHYLOXAZOLE

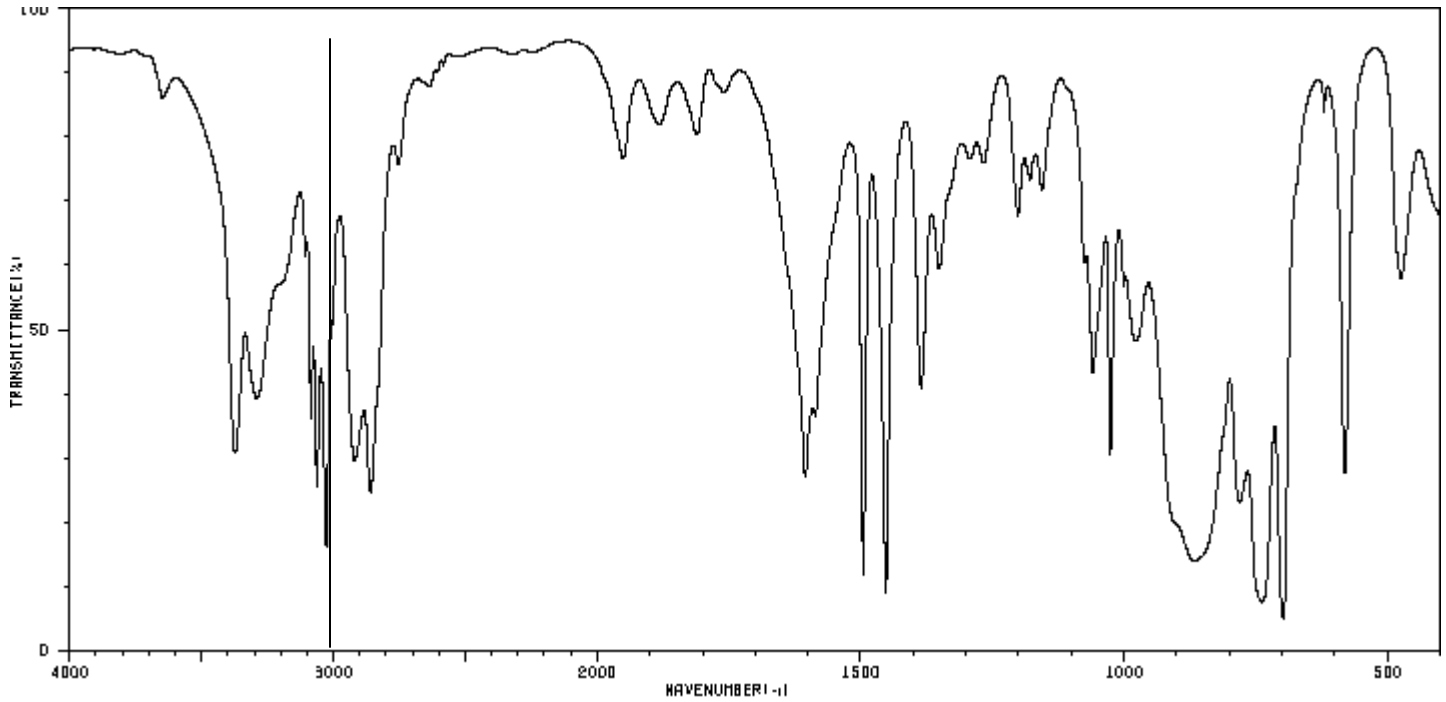
C_6H_9NO



3460	66	2766	77	1668	66	1203	14	636	27
3440	66	2582	86	1439	26	1136	33	625	81
2976	39	1719	79	1390	33	1041	66	615	61
2963	33	1709	77	1376	30	986	38	604	79
2928	14	1683	74	1352	77	931	39	597	81
2886	52	1655	26	1325	32	781	17	591	61
2863	60	1587	6	1279	4	676	49	480	81



A compound exhibits the following infrared spectrum and has a molecular weight of 107 amu. What is a likely structure for this compound?



3373	29	2869	29	1496	11	1179	70	866	13
3290	38	2753	72	1453	8	1156	68	781	22
3106	58	1950	74	1385	39	1076	58	739	7
3086	36	1881	79	1362	67	1069	42	698	4
3062	24	1810	77	1293	74	1026	29	621	81
3027	15	1605	26	1267	72	1001	55	581	26
2920	28	1586	36	1202	66	977	46	476	66

107/13 = 8.2307; 13*0.2307 = 2.999

What is the molecular formula? C_8H_{11}

C_7H_9N

How many degrees of unsaturation? 4

functional groups present: -NH; or NH_2?

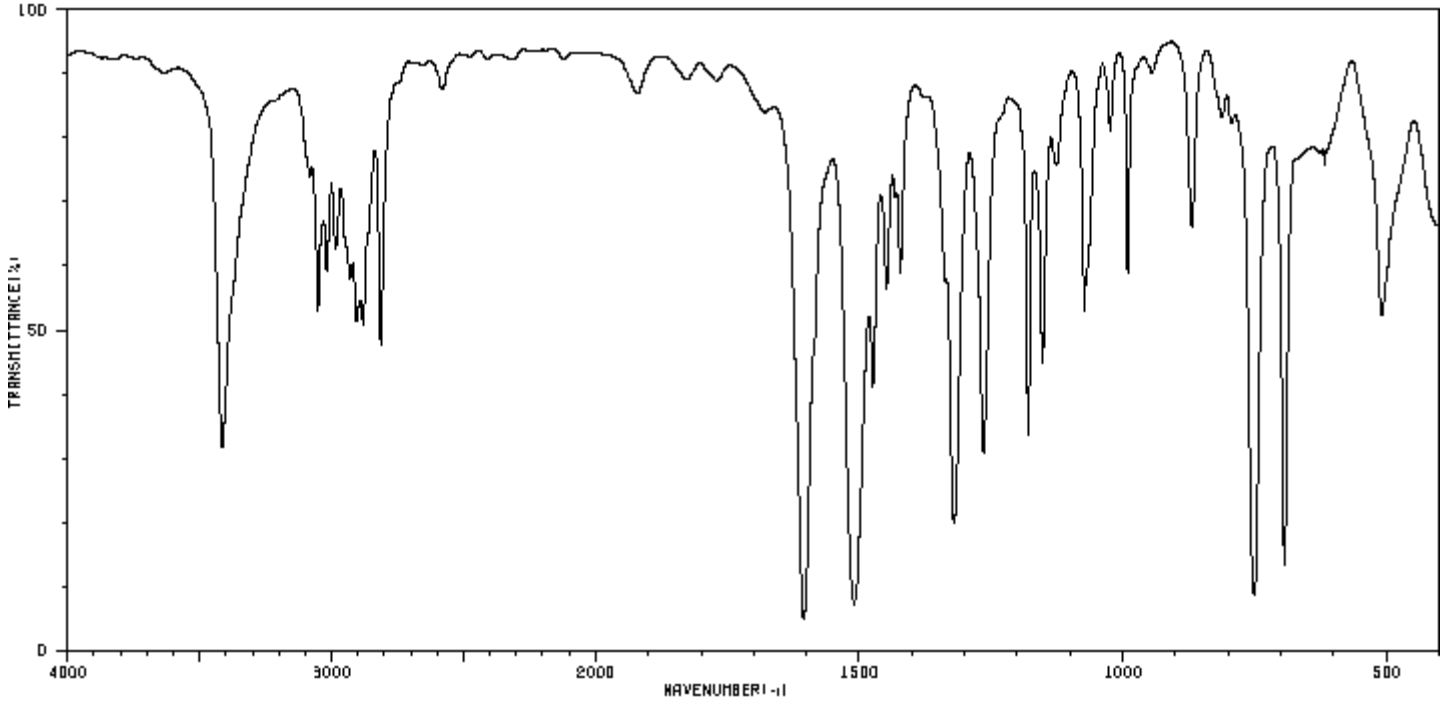
aromatic ring

possible compounds

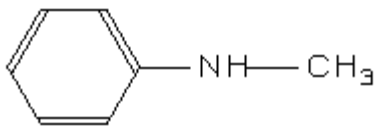
HIT-NO=1601	SCORE= ( )	SDBS-NO=1854	IR-NIDA-64365 : LIQUID FILM

N-METHYLANILINE

C_7H_9N



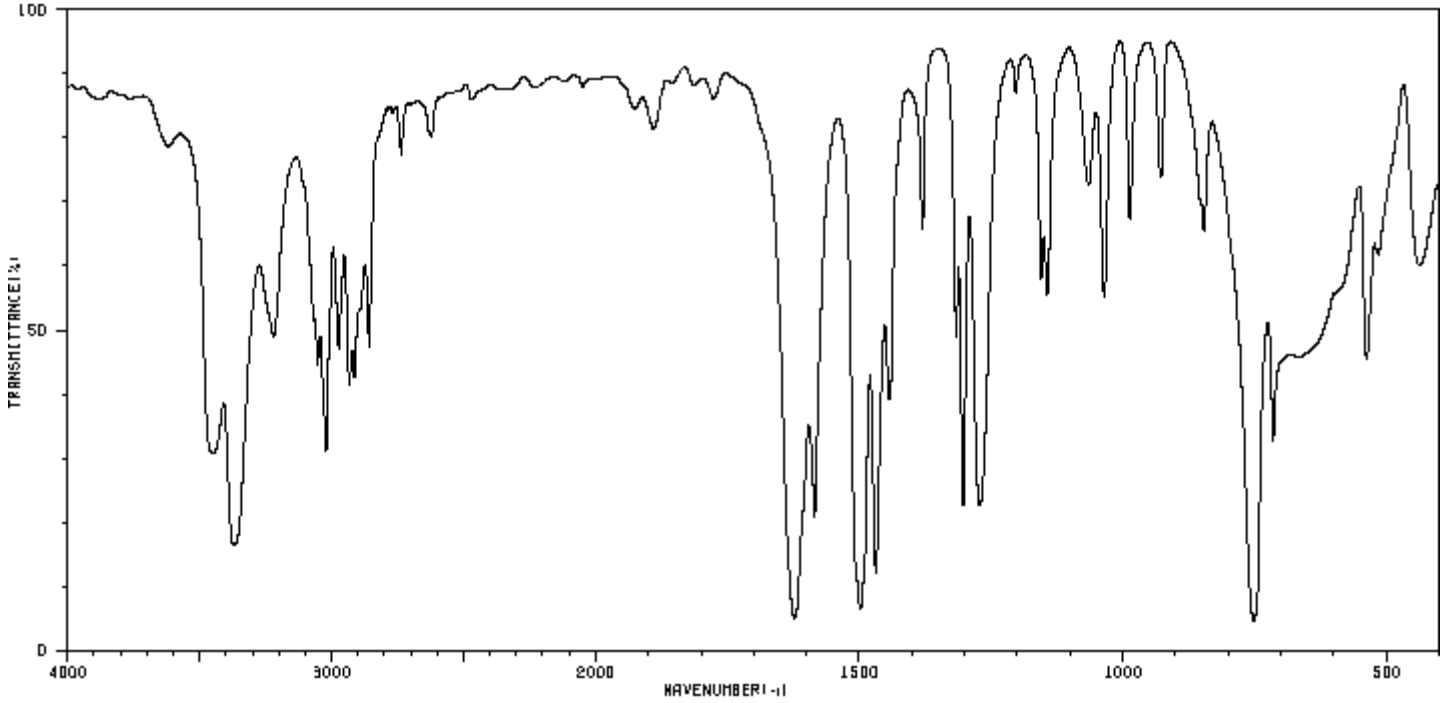
3415	31	2880	49	1610	7	1163	43	796	79
3083	72	2813	46	1474	39	1126	72	751	8
3052	52	2580	84	1446	55	1073	50	693	13
3018	67	1920	84	1422	67	1024	79	623	74
2983	60	1825	86	1320	19	991	57	617	72
2930	55	1769	86	1264	30	869	64	509	50
2906	49	1605	4	1180	32	813	79		



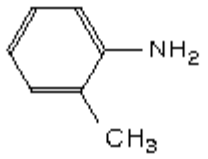
HIT-NO=1447	SCORE= ( )	SDBS-NO=1454	IR-NIDA-60212 : LIQUID FILM

O-TOLUIDINE

C_7H_9N



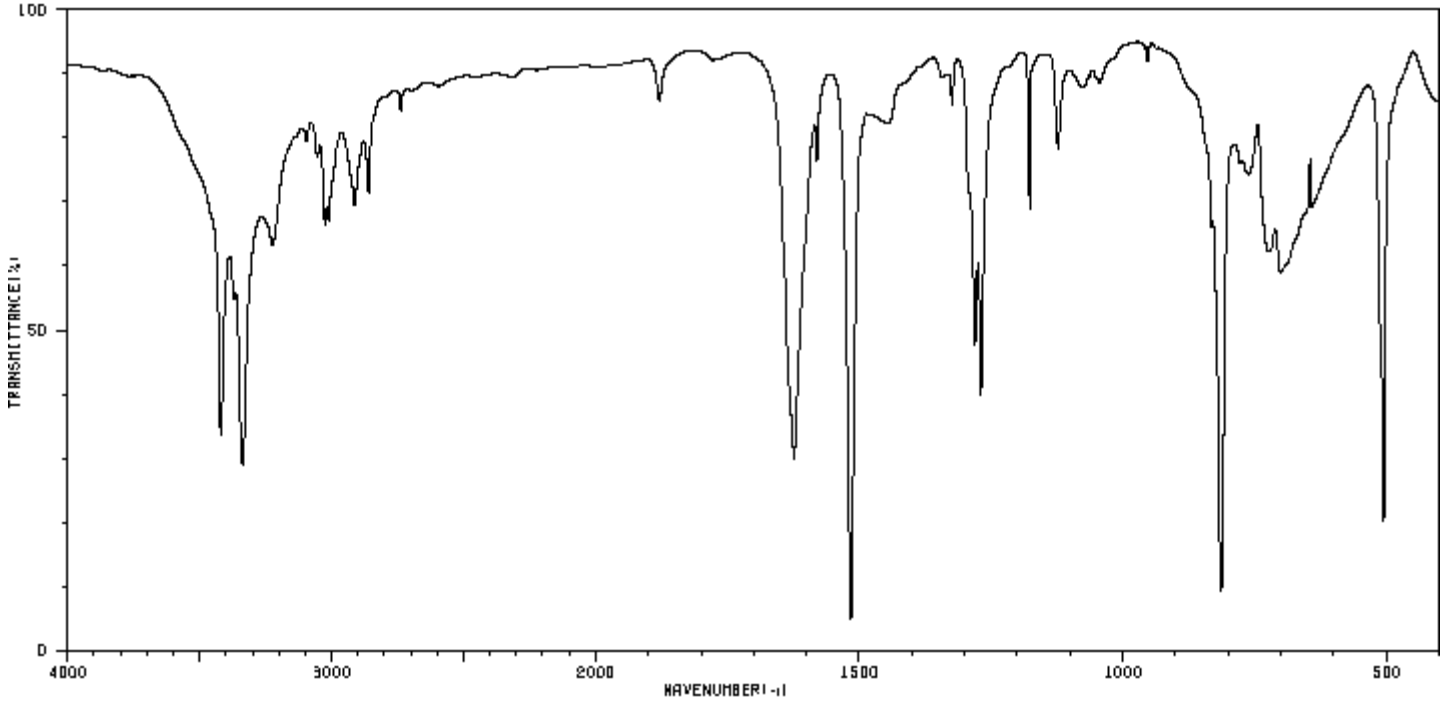
3615	77	2933	41	1686	21	1272	22	846	64
3450	30	2914	42	1498	6	1155	57	752	4
3367	16	2858	46	1469	12	1144	59	715	32
3219	47	2736	74	1443	38	1066	70	638	44
3053	43	2632	79	1380	64	1035	53	521	60
3021	31	2621	77	1317	47	987	66	516	60
2973	46	1623	6	1303	22	928	72	437	68



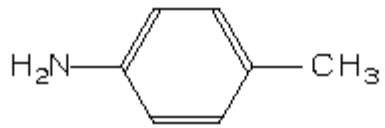
HIT-NO=1207	SCORE= ( )	SDBS-NO=990	IR-NIDA-16595 : KBR DISC

P-TOLUIDINE

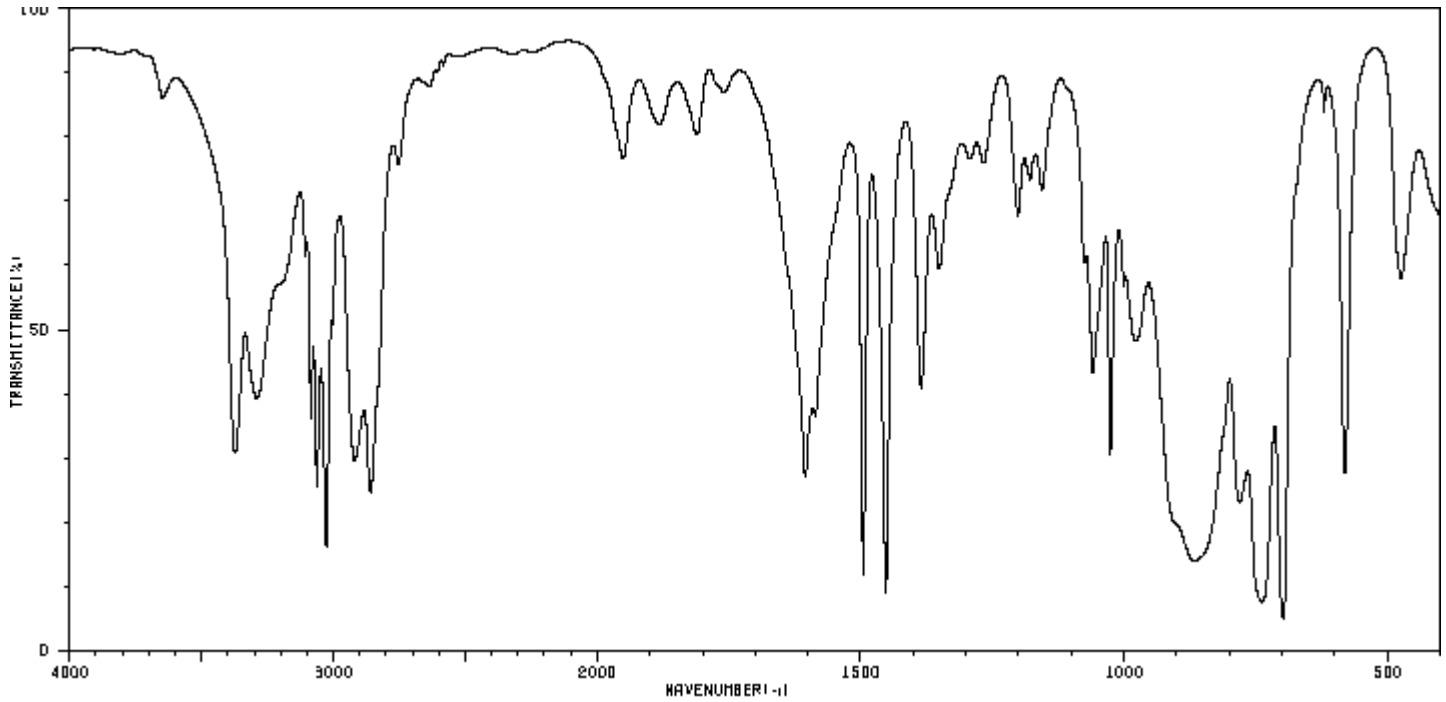
C_7H_9N



3421	32	2913	66	1463	79	1178	66	763	72
3338	27	2861	68	1446	79	1123	74	723	60
3223	60	2738	81	1344	86	1076	84	702	57
3094	77	1878	81	1332	86	1044	84	693	57
3055	74	1624	28	1324	81	813	9	642	66
3025	64	1580	74	1281	46	774	72	511	41
3011	64	1516	4	1270	38	769	72	506	19



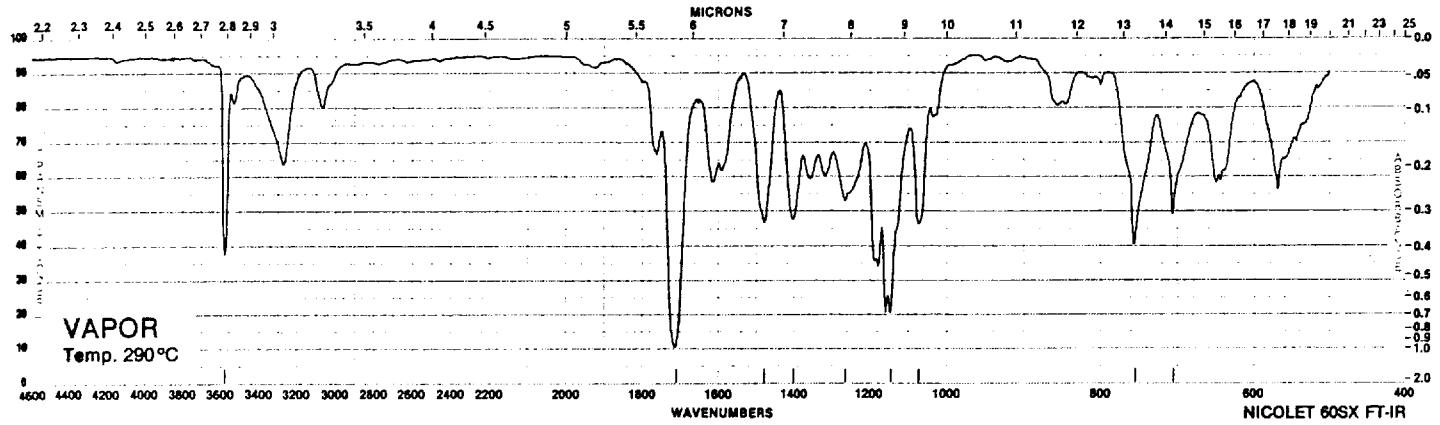
A compound exhibits the following infrared spectrum and has a molecular weight of 107 amu. What is a likely structure for this compound? benzylamine



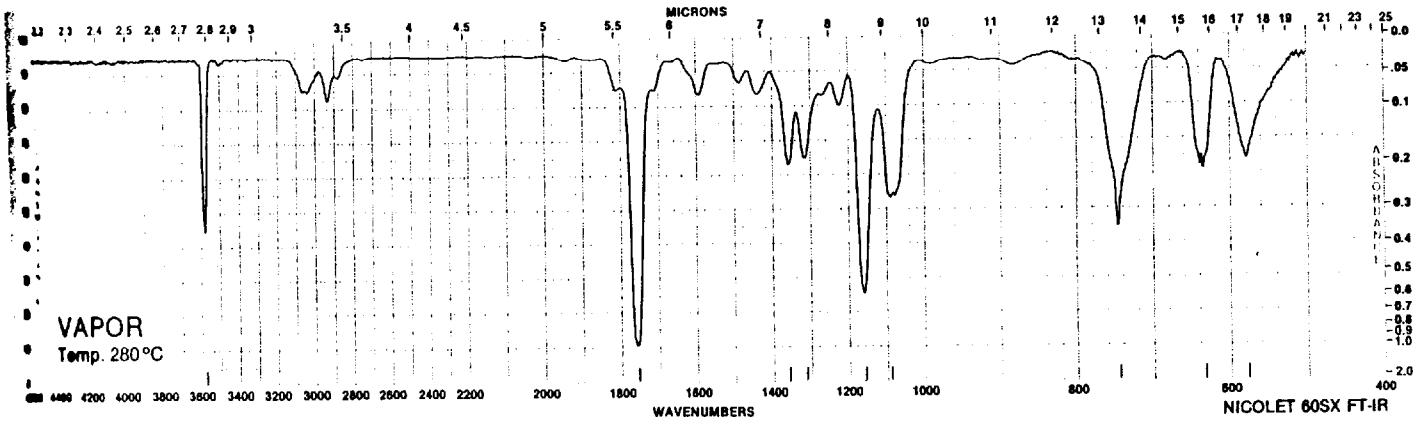
3373	29	2869	29	1496	11	1179	70	866	13
3290	38	2753	72	1453	8	1156	68	781	22
3106	58	1950	74	1385	39	1076	58	739	7
3086	36	1881	79	1362	67	1069	42	698	4
3062	24	1810	77	1293	74	1026	29	621	81
3027	15	1605	26	1267	72	1001	55	581	26
2920	28	1586	36	1202	66	977	46	476	66

4. The following are three gas phase infrared spectra for benzoic acid, 2-hydroxybenzoic acid, and 2-methoxybenzoic acid. Assign to each spectrum the correct structure and give your reasoning for each assignment.

3582.6 1403.4 1072.6
1713.1 1264.6 756.2
1480.1 1146.1 705.8

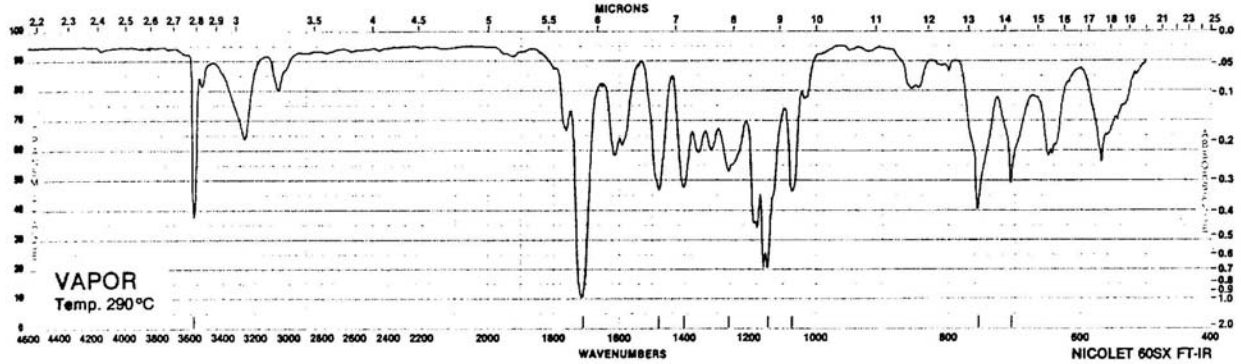


3580.8 1313.7 746.2
1759.5 1160.0 635.0
1357.8 1089.5 578.5

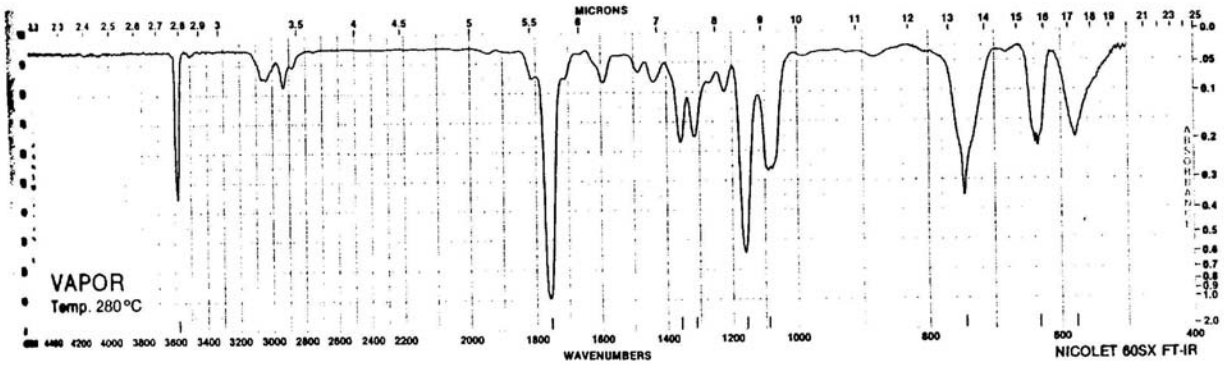


3581.0 1276.8 712.5
1767.7 1181.6 631.4
1343.3 1076.6 572.8

3582.6	1403.4	1072.6
1713.1	1264.6	756.2
1480.1	1146.1	705.8



3580.8	1313.7	746.2
1759.5	1160.0	635.0
1357.8	1089.5	578.5



3581.0	1276.8	712.5
1767.7	1181.6	631.4
1343.3	1076.6	572.8