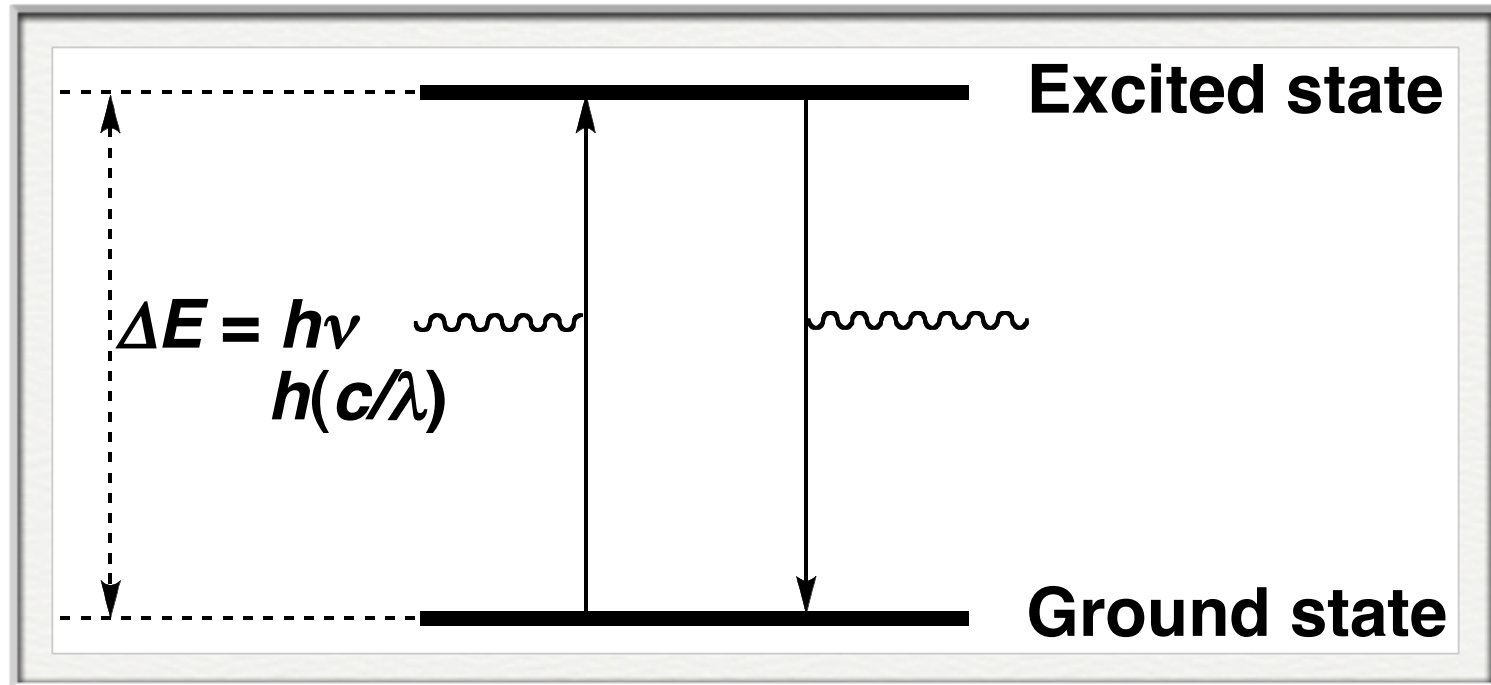


Infrared Spectroscopy (赤外分光法)

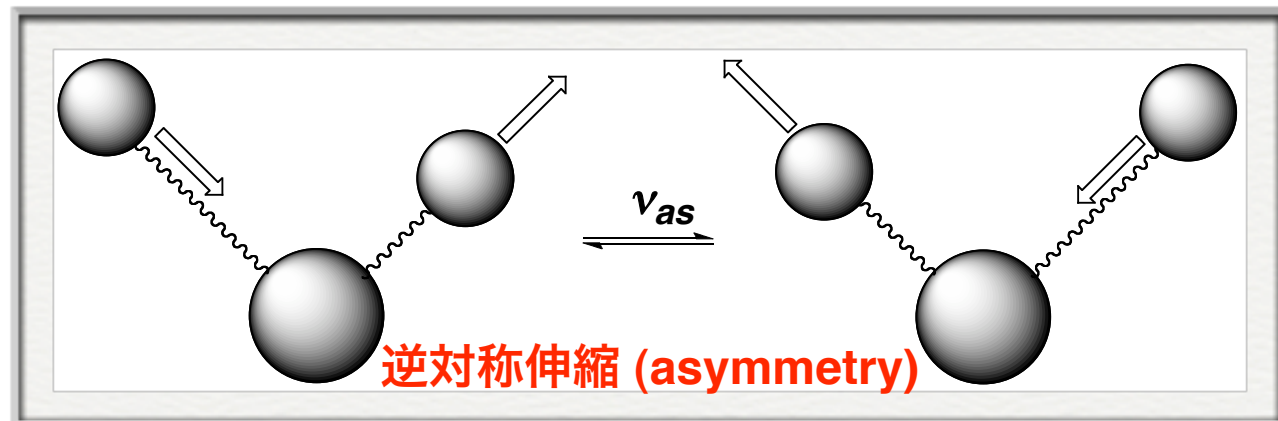
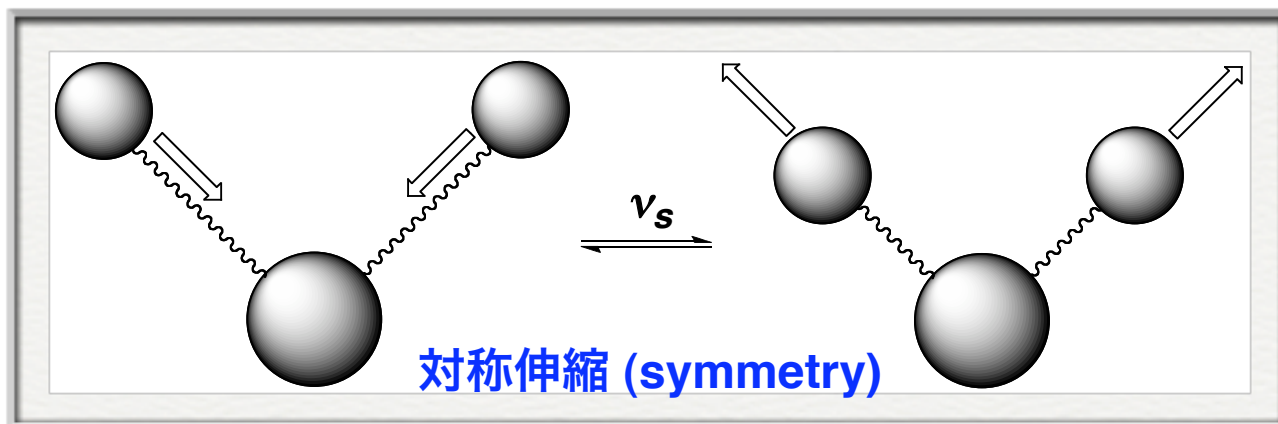
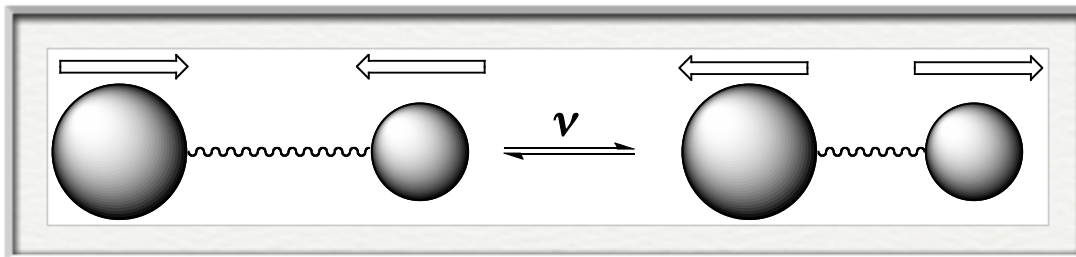
振動遷移 (vibrational transition)



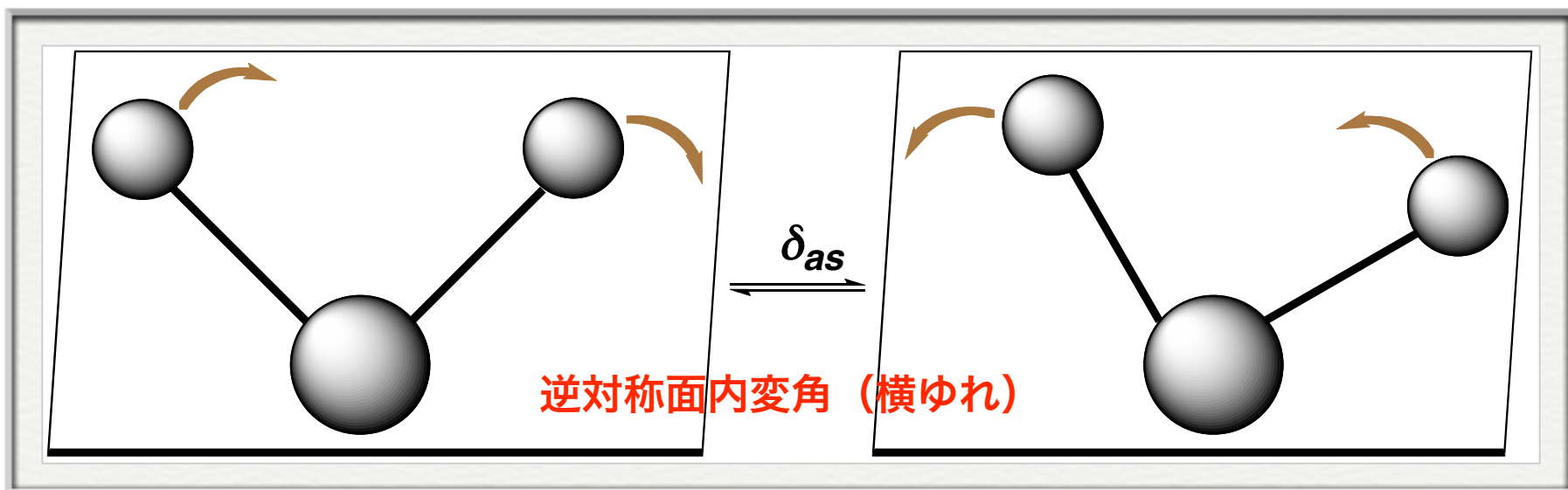
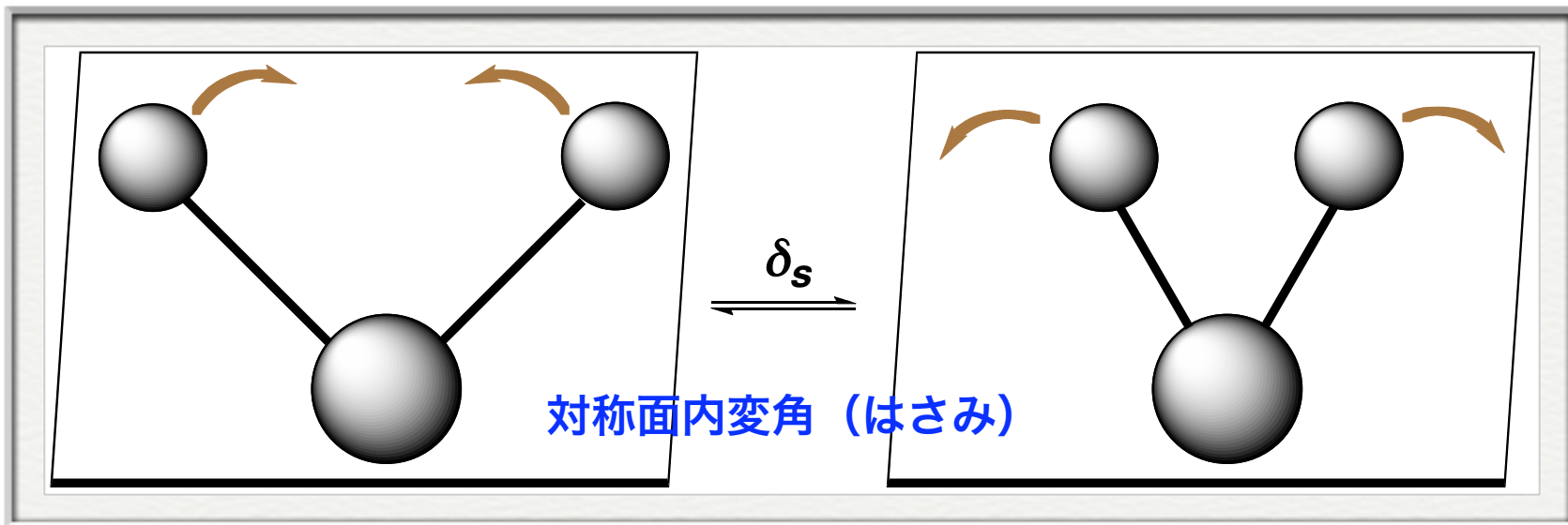
$\lambda = 2.5 \sim 25 \mu\text{m}$ 赤外線

$\frac{1}{\lambda} = \tilde{\nu} = 4000 \sim 400 \text{ cm}^{-1}$... 波数 または カイザー

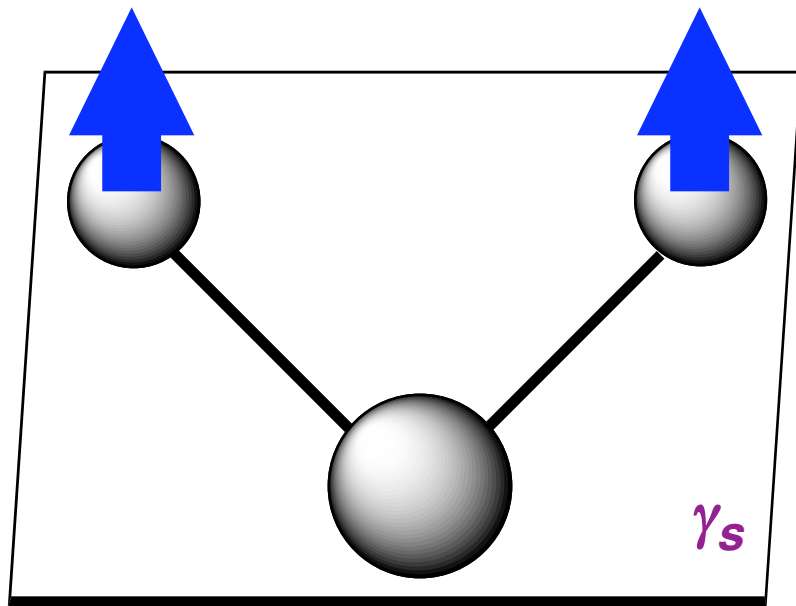
伸縮振動 (stretching)



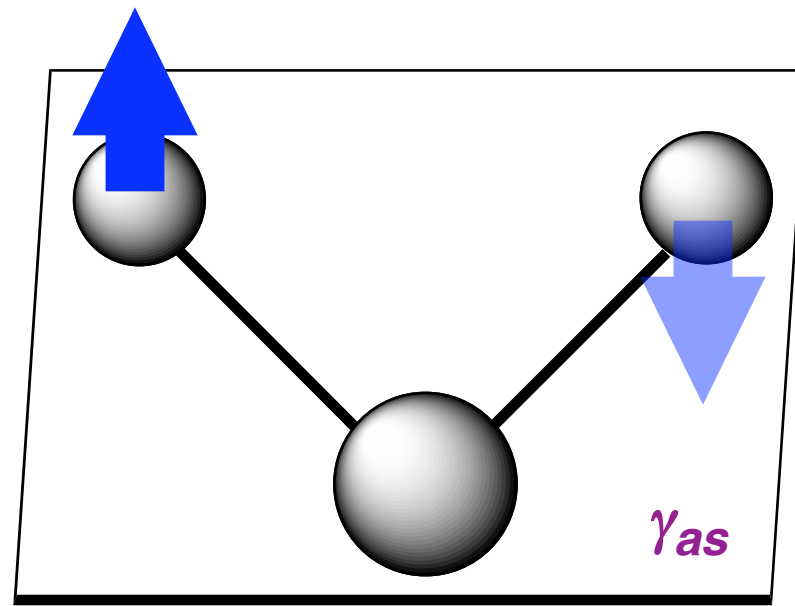
面内変角振動 (vending)



面外変角振動 (vending)



対称面外変角 (縦揺れ)



逆対称面外変角 (ひねり)

吸収波数（フックの法則）

結合のポテンシャルエネルギー: $V(r) = \frac{1}{2}kx^2$

k : 力の定数 \approx 結合の強さ

結合の振動数: $\tilde{\nu} = \frac{1}{2\pi} \sqrt{\frac{k}{\mu}}$, $\mu = \frac{m_1 m_2}{m_1 + m_2}$ (換算質量)

ポイント (μ と k の兼ね合い)

1. $\tilde{\nu}$ (stretching) > $\tilde{\nu}$ (bending)

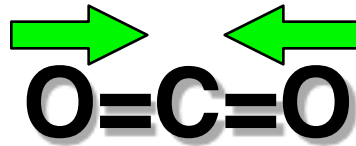
2. $\tilde{\nu}$ (C \equiv C) > $\tilde{\nu}$ (C=C) > $\tilde{\nu}$ (C-C)

3. $\tilde{\nu}$ (C-H) > $\tilde{\nu}$ (C-C), $\tilde{\nu}$ (O-H) > $\tilde{\nu}$ (C-O), $\tilde{\nu}$ (O-H) > $\tilde{\nu}$ (C-H)

吸収強度 (遷移確率)



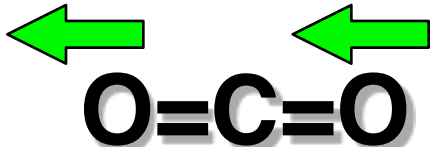
赤外不活性 (ラマン活性)



双極子モーメントの変化無し

禁制遷移

対称伸縮やはさみ振動は弱い

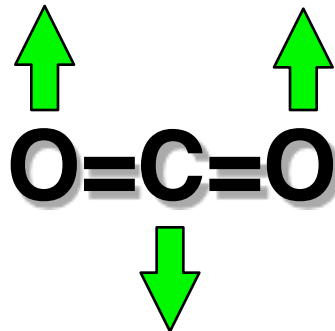


赤外活性 (ラマン不活性)



双極子モーメントが変化

許容遷移



赤外活性 (ラマン不活性)

C-O伸縮はC-C伸縮より高波数

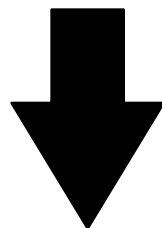
C=O伸縮はC=C伸縮より高波数

官能基と特性吸収

非直線分子 (N原子) の基準振動の数: $3N-6$

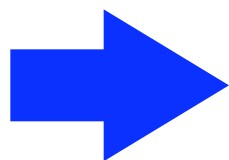
直線分子 (N原子) の基準振動の数: $3N-5$

例) メタン (CH_4): $3 \times 5 - 6 = 9$; エタン (C_2H_6): $3 \times 8 - 6 = 18$



+ 縮重
+ 倍音 (弱い)
+ 結合音 (弱い)

一般にIRスペクトルは非常に複雑 (全てのピークの帰属は不可能)
普遍的に存在するC-CやC-H結合に由来するピークは、あまり役に立たない。



官能基の特性吸収に注目 (例えばC=O)

試料の調製

測定条件は、吸収位置に影響（特に水素結合）

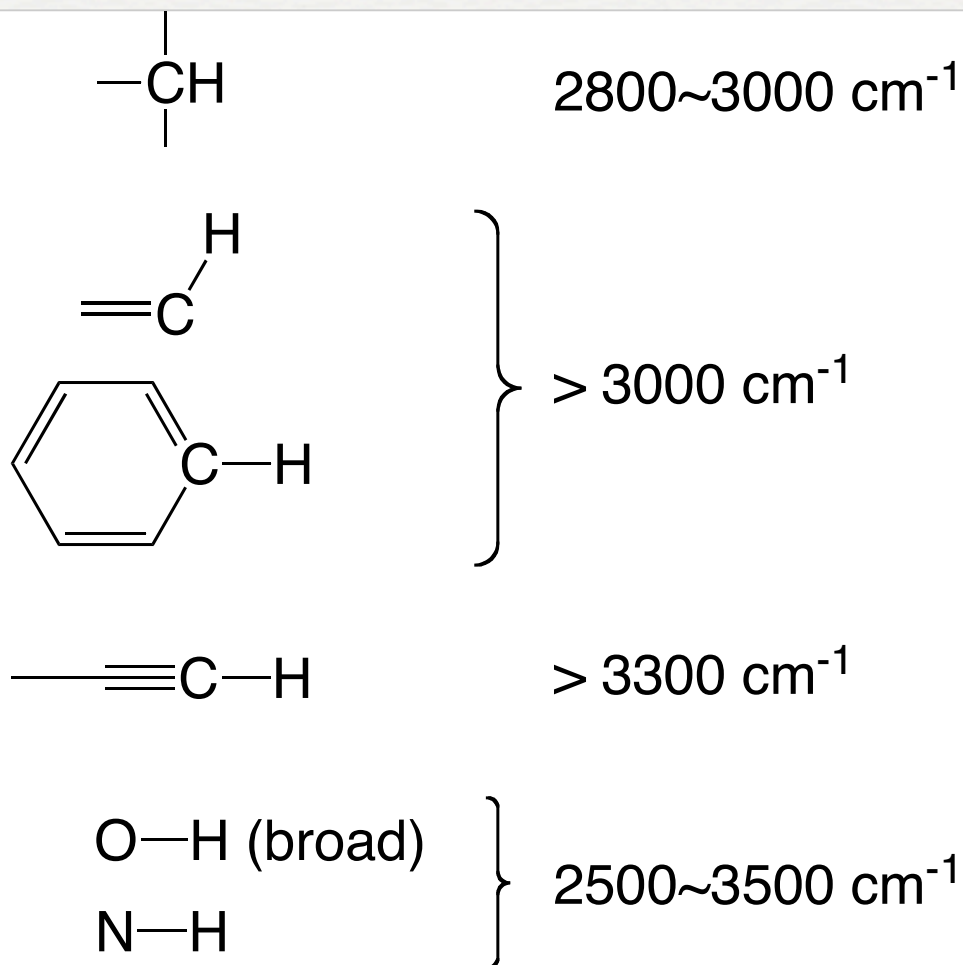
溶液 ☞ NaCl板

液体 ☞ NaCl板, Nujol (炭化水素), (KBrディスク)

個体 ☞ KBrディスク, Nujol

ガラス、石英、プラスチックは不可

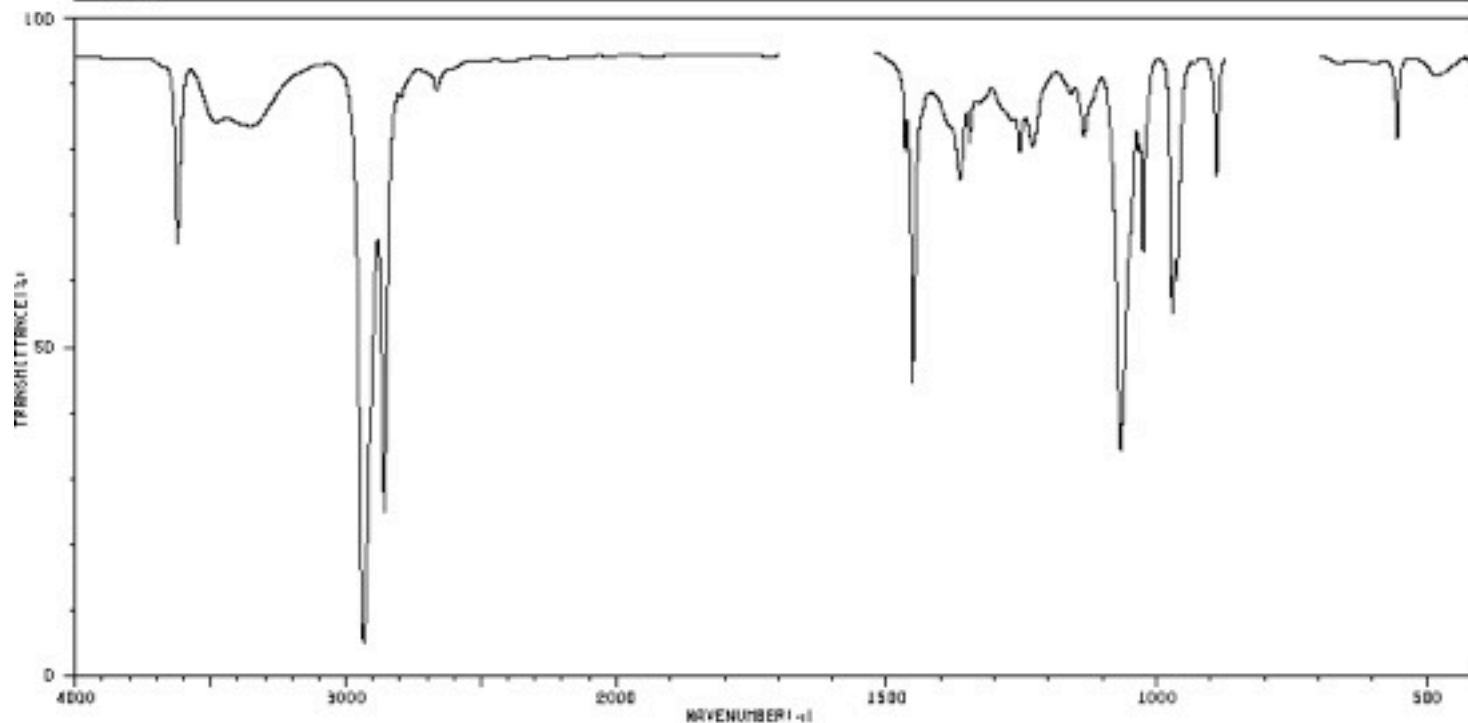
4000 cm^{-1} ~ 2500 cm^{-1}
(O-H, N-H, C-H伸縮)



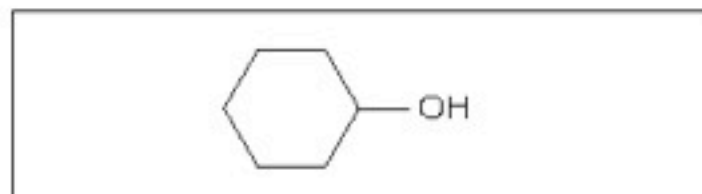
結合の強さを反映

アルコールのO-H伸縮振動 (solution)

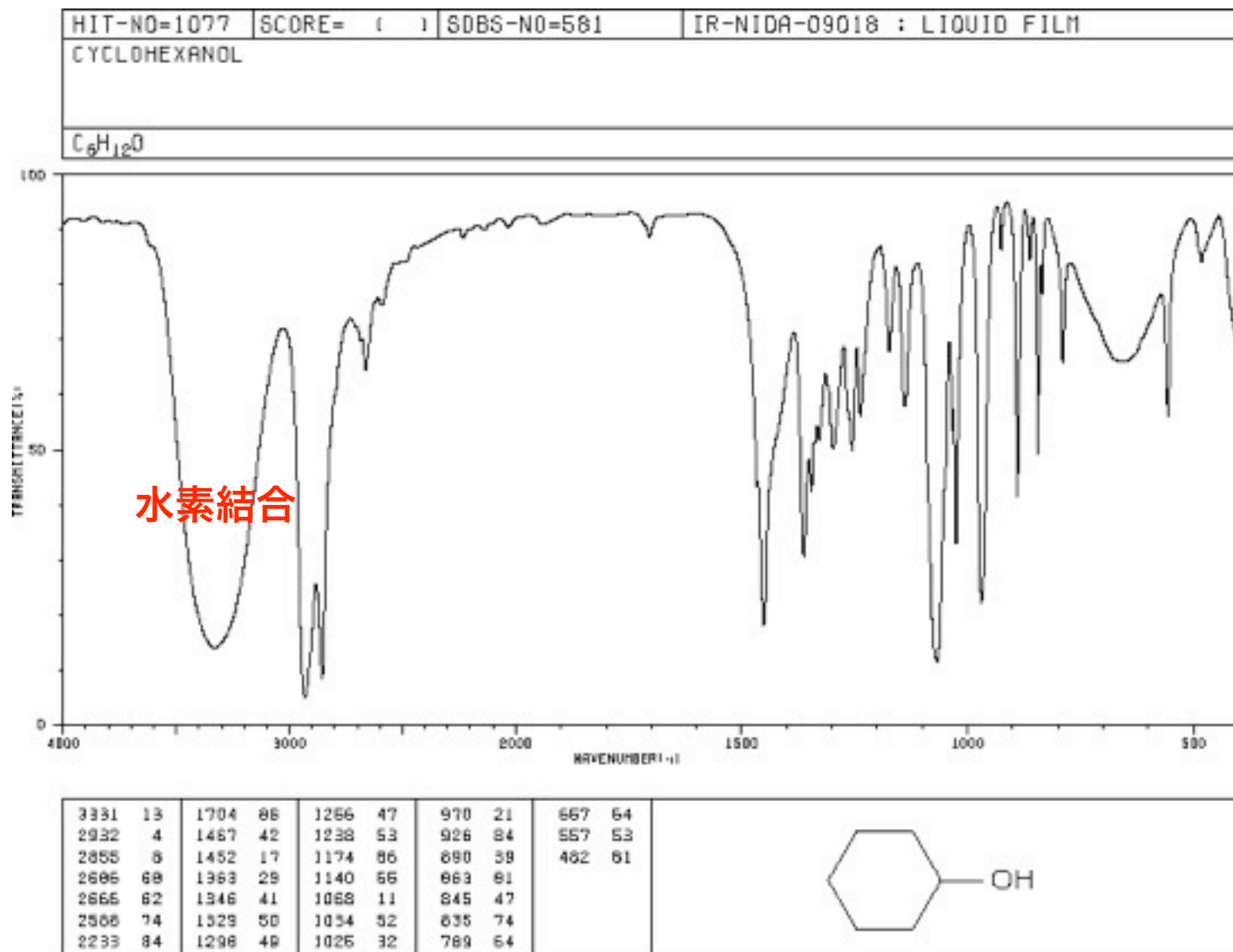
HIT-NO=968	SCORE= ()	SDBS-NO=581	IR-NIDA-08688 : CCL4 SOLUTION
CYCLOHEXANOL			
C ₆ H ₁₂ O			



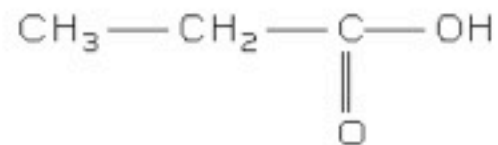
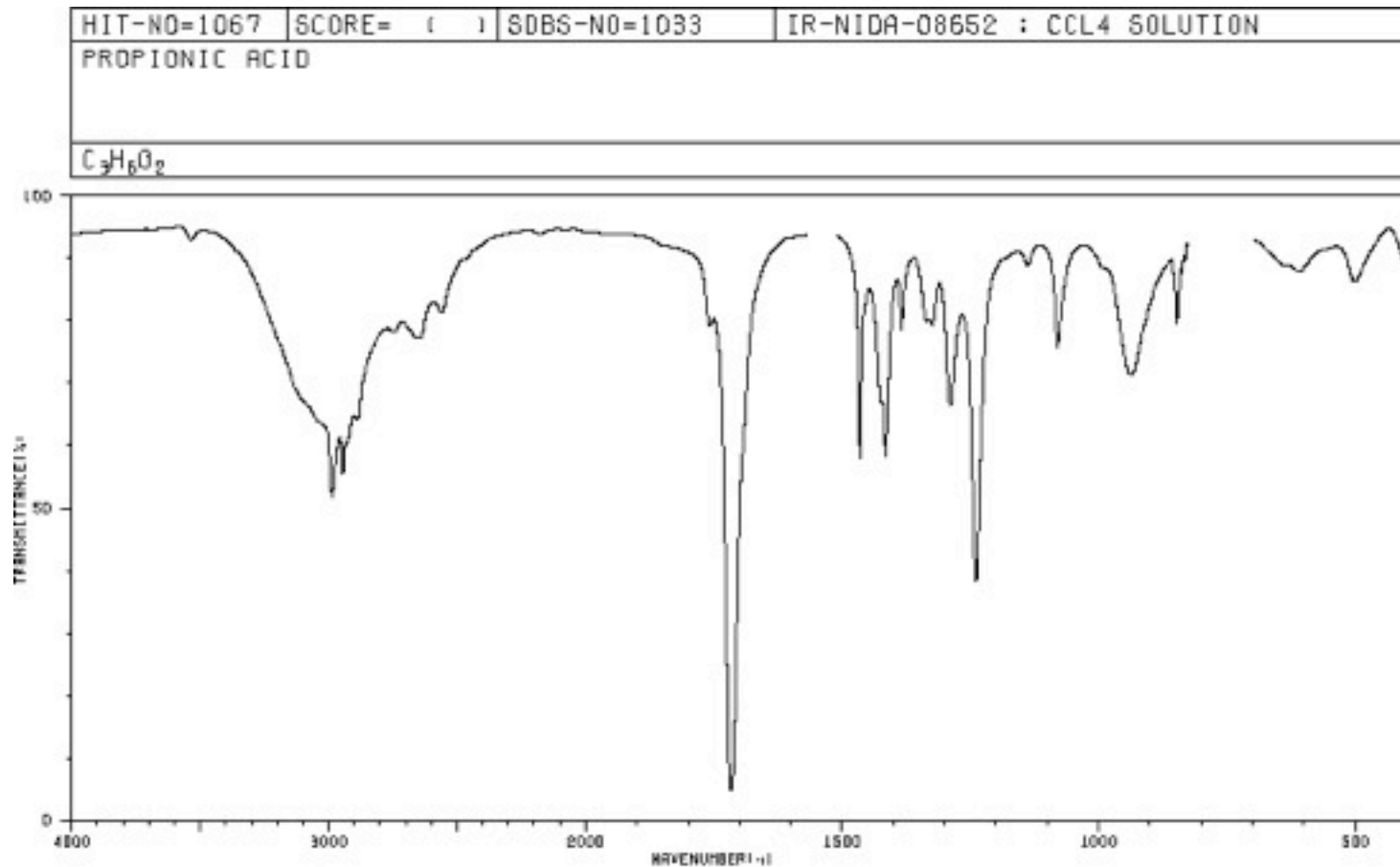
3623	62	1347	79	971	63
2934	4	1254	77	963	58
2858	23	1230	77	889	72
2866	86	1160	84	666	79
1466	77	1135	79		
1455	43	1067	39		
1366	72	1026	62		



アルコールのO-H伸縮振動 (neat)

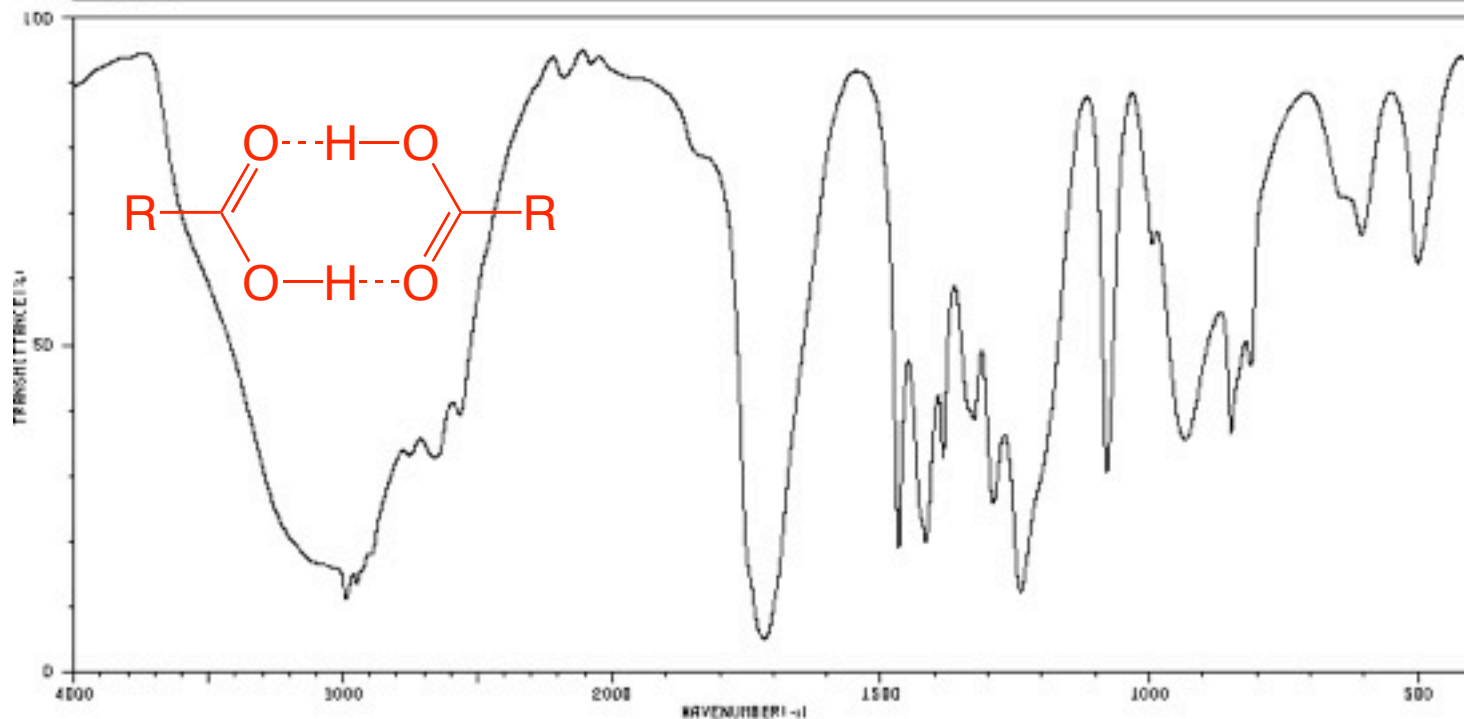


カルボン酸のO-H伸縮振動 (solution)

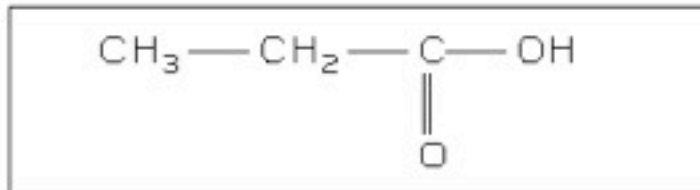


カルボン酸のO-H伸縮振動 (liquid film)

HIT-NO=1276 SCORE= () SDBS-NO=1033 IR-NIDA-05127 ; LIQUID FILM
 PROPIONIC ACID
 $C_3H_6O_2$

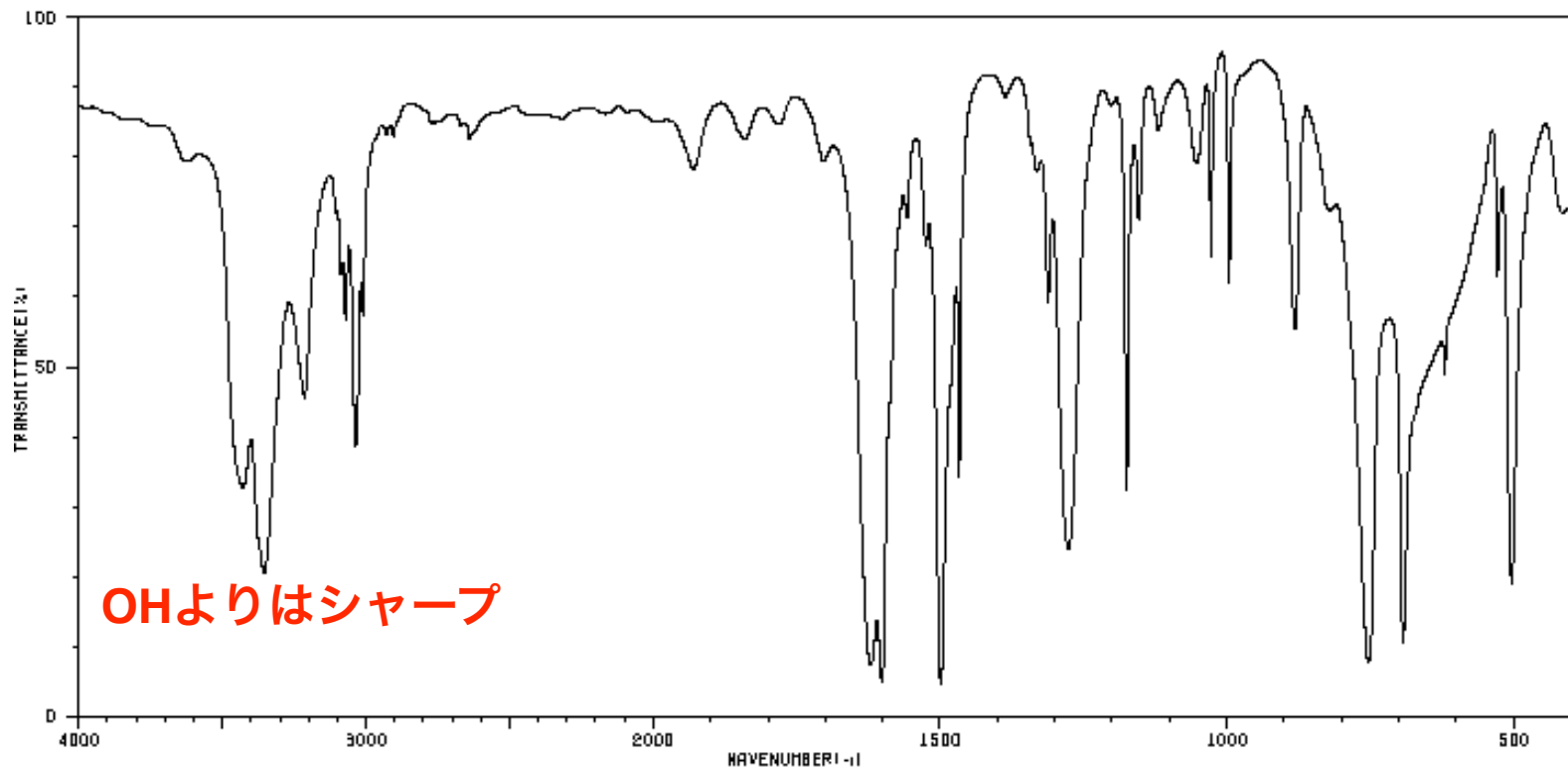


2966	10	1304	32	848	36
2948	12	1327	37	811	44
2860	31	1291	25	814	86
2666	38	1240	12	606	64
1716	4	1080	29	501	60
1467	16	995	62		
1416	19	933	34		

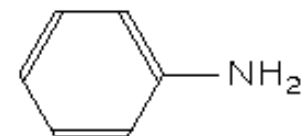


N-H伸縮振動 (primary amine)

HIT-NO=1244	SCORE= ()	SDBS-NO=905	IR-NIDA-15056 : LIQUID FILM
ANILINE			
C ₆ H ₇ N			

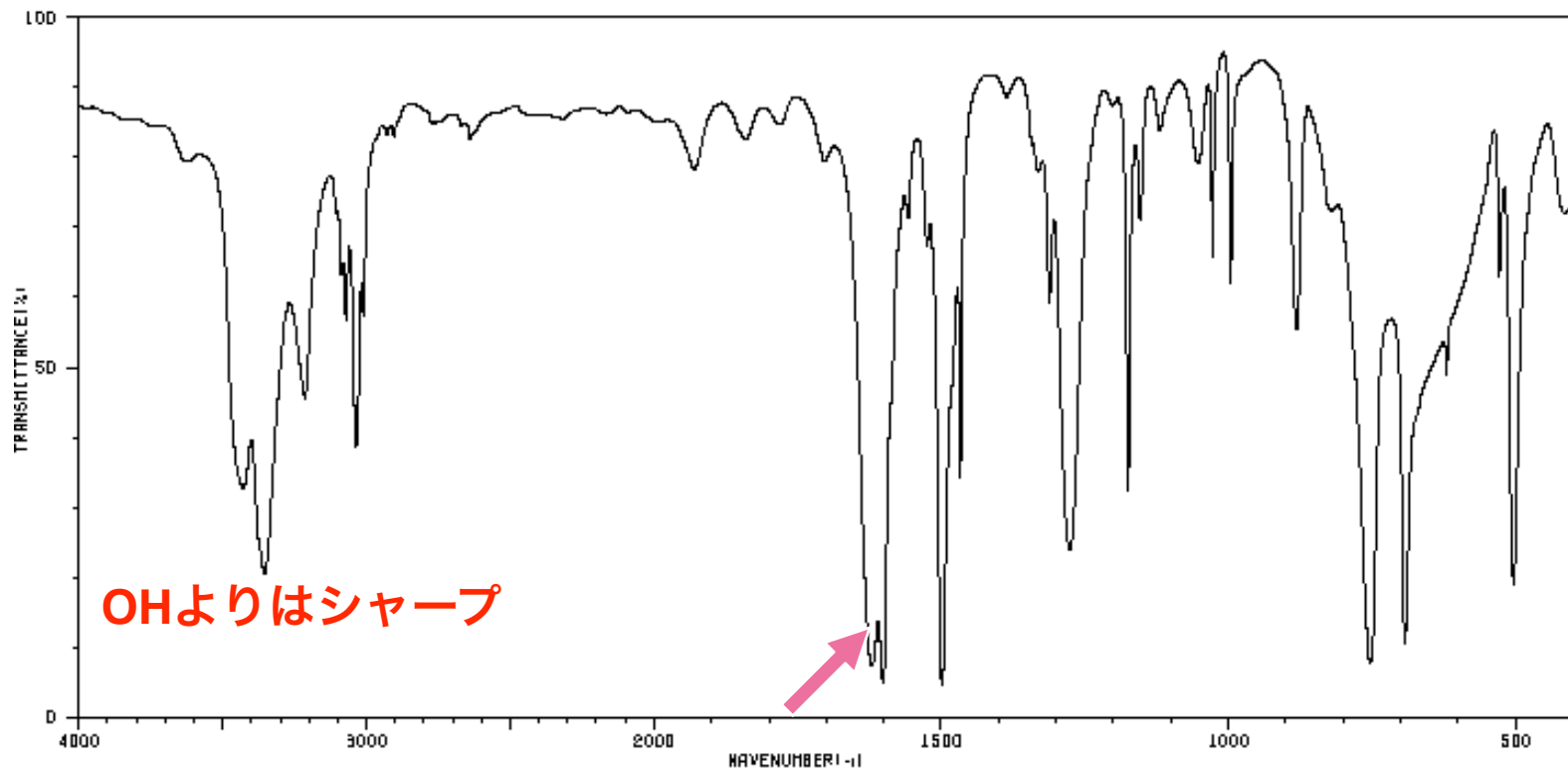


3623	77	3010	67	1705	77	1332	74	996	60
3429	32	2930	81	1621	7	1312	57	881	53
3354	20	2904	79	1801	5	1277	29	754	8
3214	44	2640	79	1667	70	1176	32	693	10
3088	62	2627	81	1525	66	1154	68	620	47
3072	55	1929	77	1498	4	1053	77	529	60
3037	38	1839	79	1467	34	1028	64	504	18

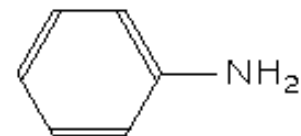


N-H伸縮振動 (primary amine)

HIT-NO=1244	SCORE= ()	SDBS-NO=905	IR-NIDA-15056 : LIQUID FILM
ANILINE			
C ₆ H ₇ N			

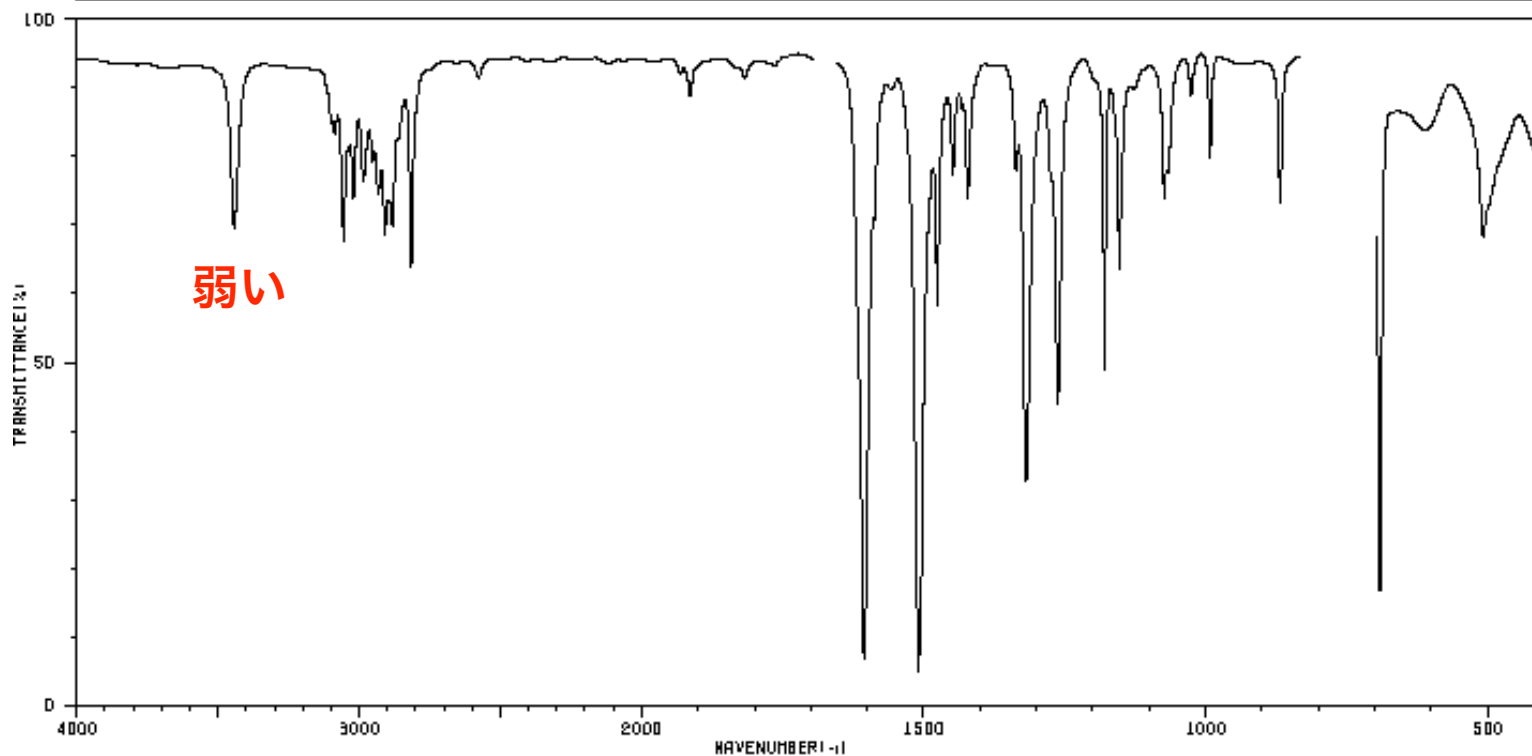


3623	77	3010	67	1705	77	1332	74	996	60
3429	32	2930	81	1621	7	1312	57	881	53
3354	20	2904	79	1801	5	1277	29	754	8
3214	44	2640	79	1667	70	1176	32	693	10
3088	62	2627	81	1525	66	1154	68	620	47
3072	55	1929	77	1498	4	1053	77	529	60
3037	38	1839	79	1467	34	1028	64	504	18



N-H伸縮振動 (secondary amine)

HIT-NO=1472	SCORE= ()	SDBS-NO=1854	IR-NIDA-06920 : CCL4 SOLUTION
N-METHYLANILINE			
C ₇ H ₉ N			

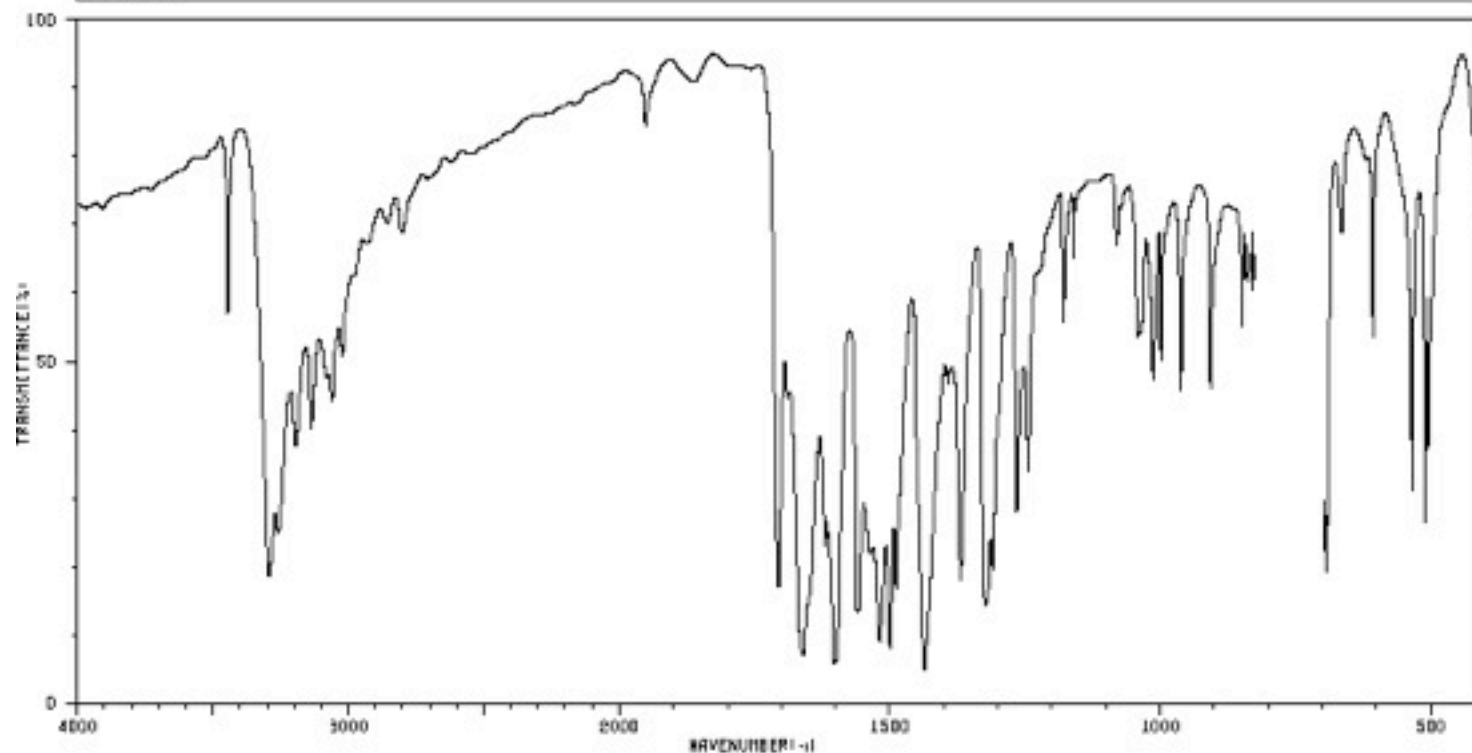


3443	66	2932	72	1806	6	1319	31	992	77
3098	81	2909	66	1509	4	1262	42	868	70
3086	79	2882	66	1476	55	1180	47	691	16
3066	64	2816	62	1449	74	1164	60	618	81
3021	70	1914	86	1433	84	1074	70	610	81
2985	74	1677	95	1422	70	1067	74	509	66
2963	77	1672	96	1337	74	1026	86		

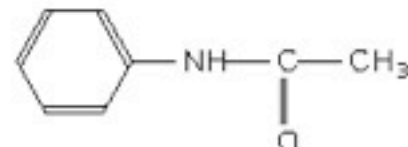
CNc1ccccc1

N-H伸縮振動 (solution)

HIT-NO=1123	SCORE= ()	SOBS-NO=729	IR-NIDA-08648 : CCL4 SOLUTION
ACETANILIDE			
C ₈ H ₉ NO			

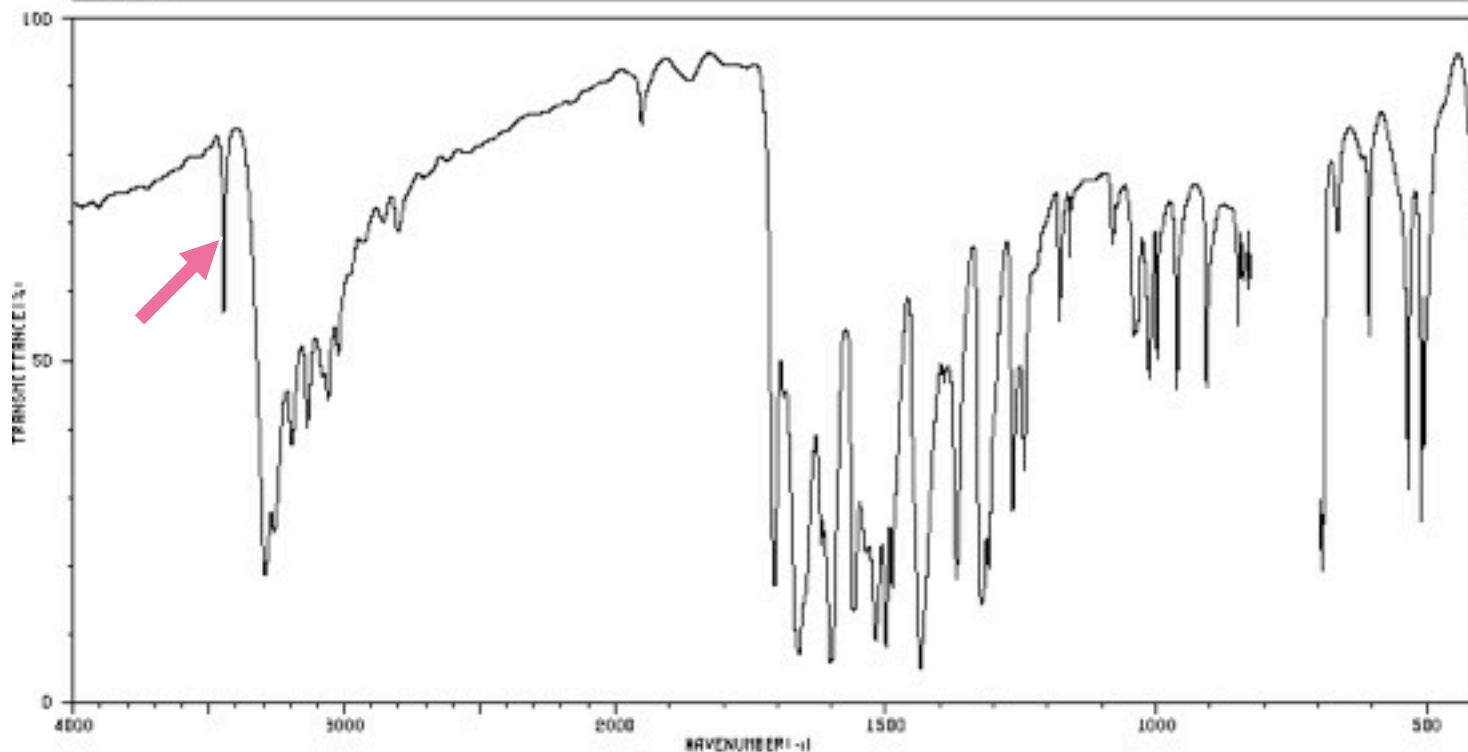


3445	55	3022	49	1499	7	1265	26	907	44
3292	17	1708	18	1489	16	1244	32	849	53
3258	23	1661	6	1457	4	1180	58	694	18
3193	36	1620	21	1393	44	1042	62	607	62
3136	38	1603	5	1370	17	1013	46	535	30
3080	46	1560	13	1324	13	999	47	511	25
3060	42	1519	8	1310	18	962	44	506	35

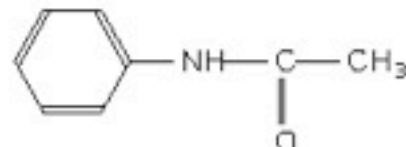


N-H伸縮振動 (solution)

HIT-NO=1123	SCORE= ()	SOBS-NO=729	IR-NIDA-08648 : CCL4 SOLUTION
ACETANILIDE			
C ₈ H ₉ NO			

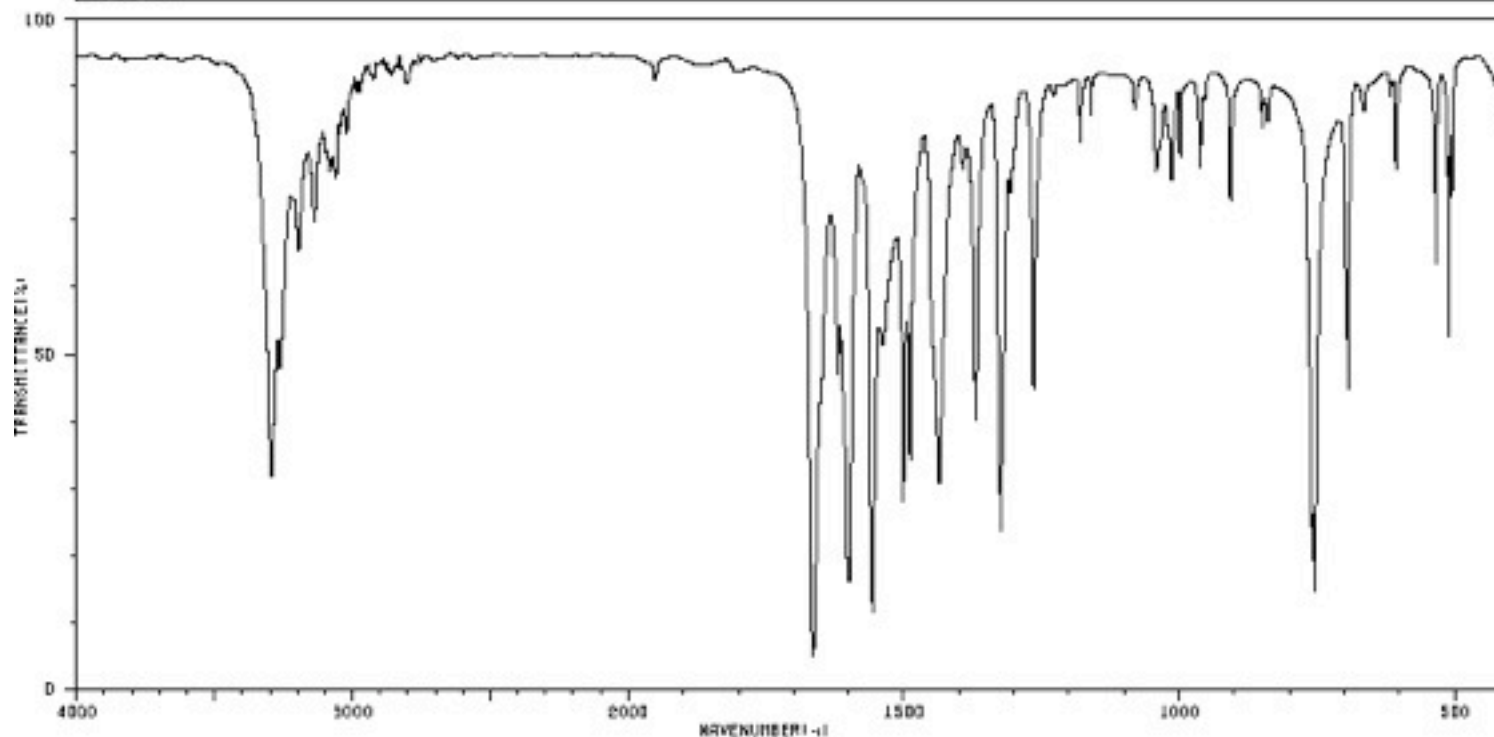


3445	55	3022	49	1499	7	1265	26	907	44
3292	17	1708	18	1489	16	1244	32	849	53
3258	23	1661	6	1457	4	1180	58	694	18
3193	36	1620	21	1393	44	1042	62	607	62
3136	38	1603	5	1370	17	1013	46	535	30
3080	46	1560	13	1324	13	999	47	511	25
3060	42	1519	8	1310	18	962	44	606	35

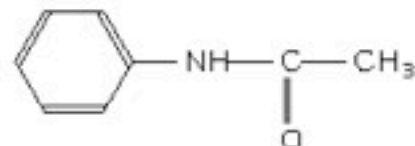


N-H伸縮振動 (KBr)

HIT-NO=1095	SCORE= ()	S0BS-NO=729	IR-NIDA-61373 ; KBR DISC
ACETANILIDE			
C ₈ H ₉ NO			

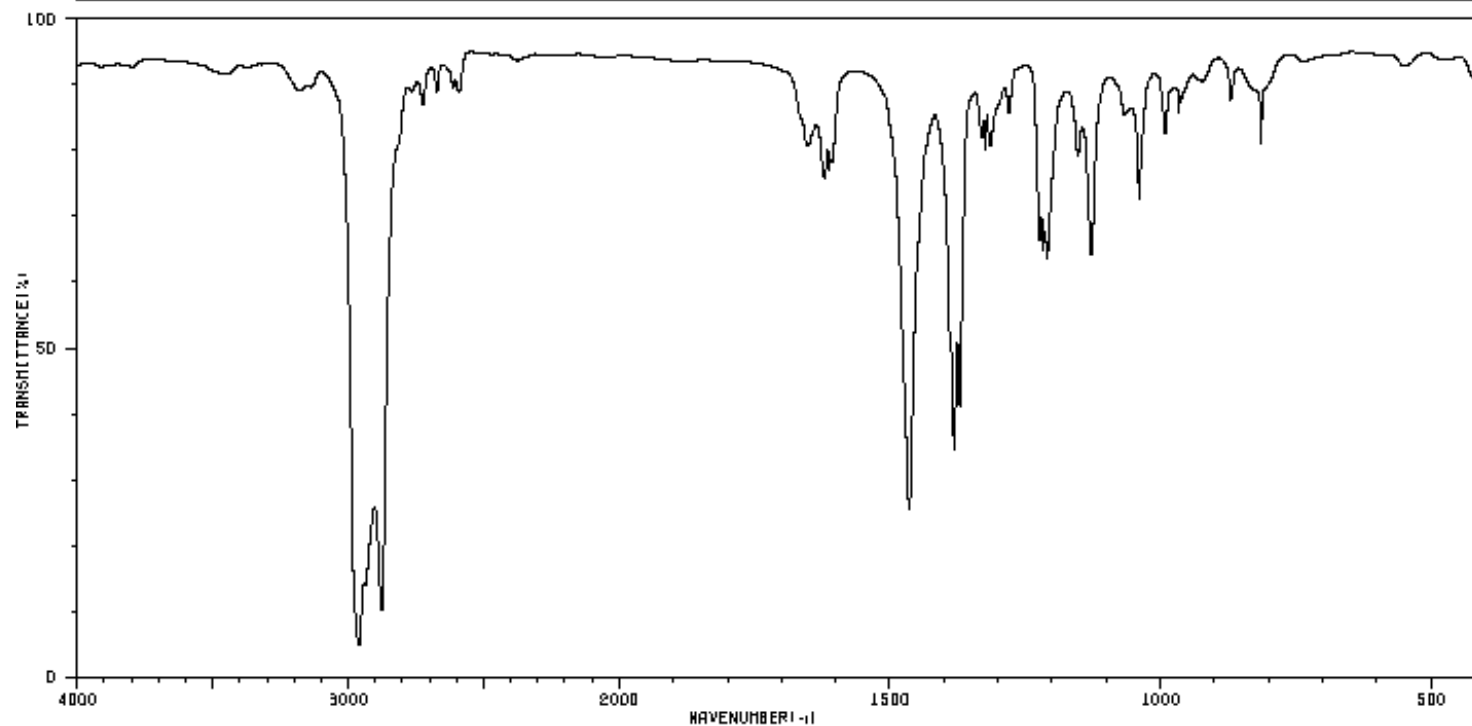


3294	30	3022	79	1489	33	1180	79	761	23
3261	46	1665	4	1436	29	1042	74	754	13
3196	82	1620	44	1393	74	1014	72	694	43
3137	66	1699	16	1369	38	999	77	607	74
3083	74	1557	10	1324	22	962	74	534	60
3059	74	1538	49	1307	72	908	70	511	50
3046	79	1601	28	1266	43	768	62	606	70

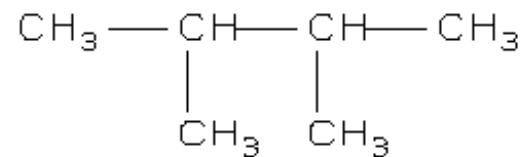


C(sp³)-H伸縮振動 (アルカン)

HIT-NO=1104	SCORE= ()	SDBS-NO=654	IR-NIDA-02888 : LIQUID FILM
2,3-DIMETHYLBUTANE			
C ₆ H ₁₄			

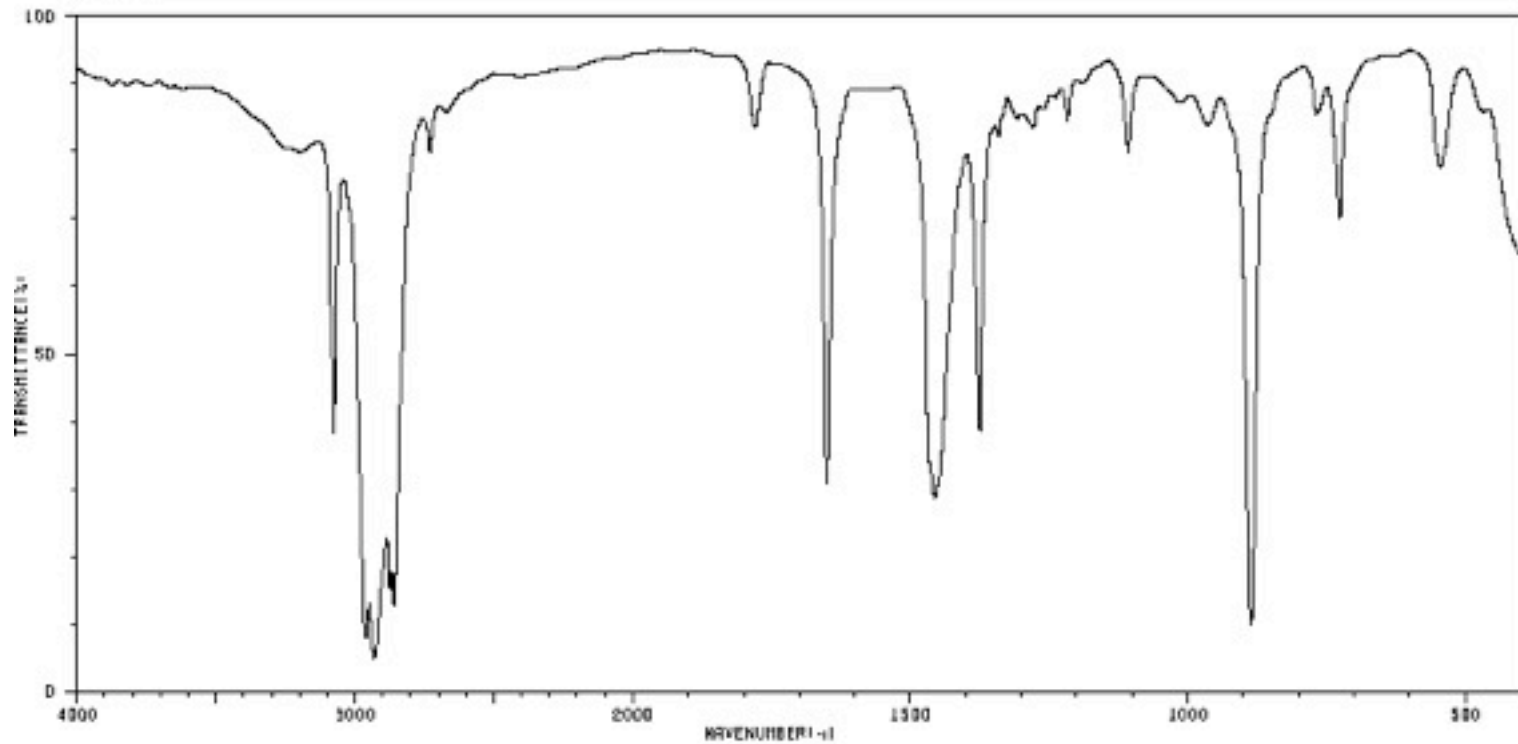


3176	86	2951	86	1381	33	1218	62	960	84
2959	4	1651	77	1371	39	1209	60	870	84
2936	13	1621	72	1330	79	1153	77	823	86
2876	9	1613	74	1323	77	1128	62	814	79
2722	84	1607	74	1315	77	1039	70		
2673	86	1464	24	1280	81	991	78		
2614	86	1389	48	1223	64	966	81		

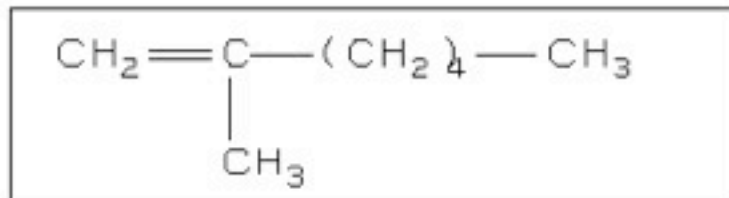


C(sp²)-H伸縮振動

HIT-NO=3282 | SCORE= () | SDBS-NO=6239 | IR-NIDA-10670 ; LIQUID FILM
2-METHYL-1-HEPTENE
C₈H₁₆

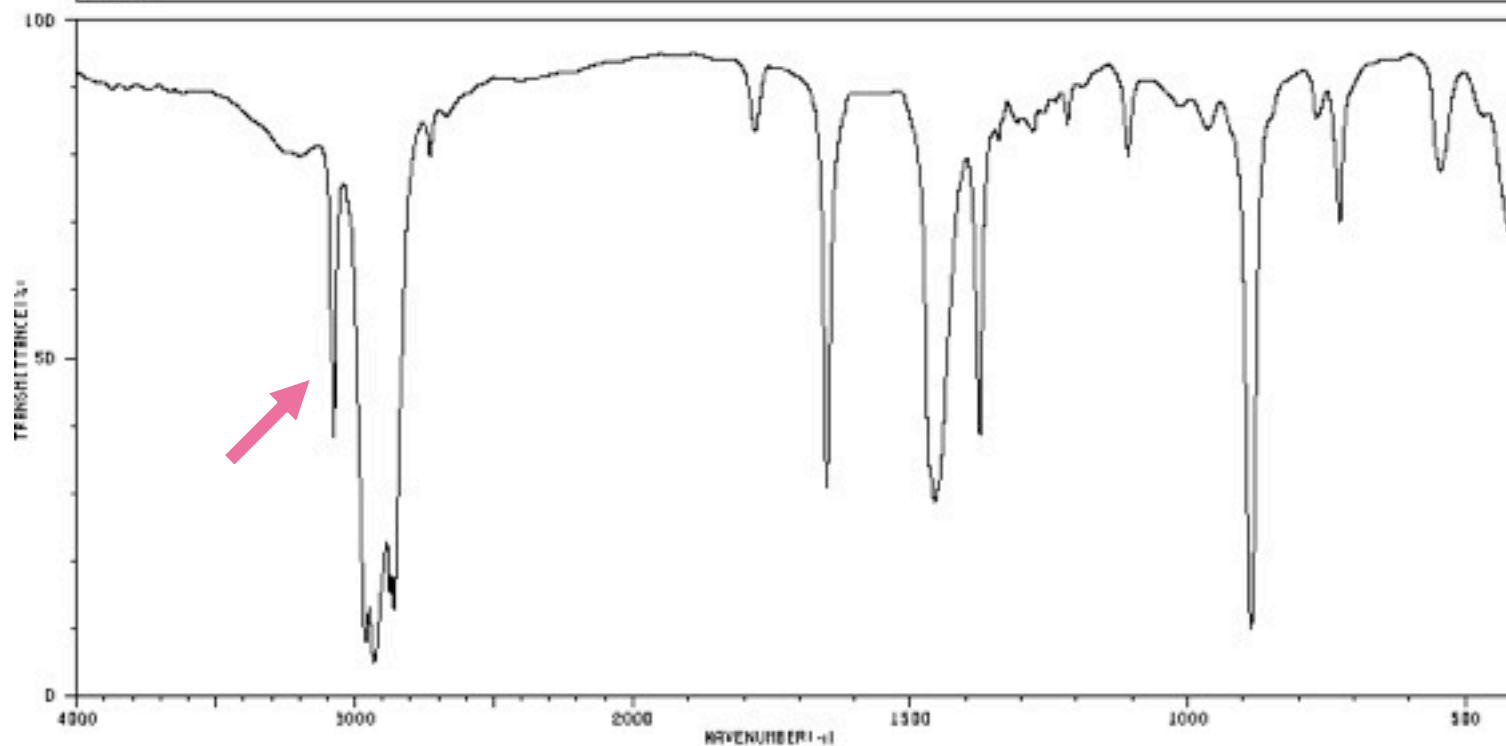


3076	37	1661	29	1108	77
2960	7	1458	27	963	81
2930	4	1375	37	886	9
2874	14	1341	79	769	81
2861	12	1294	81	726	68
2729	77	1278	79	546	74
1780	81	1217	81		

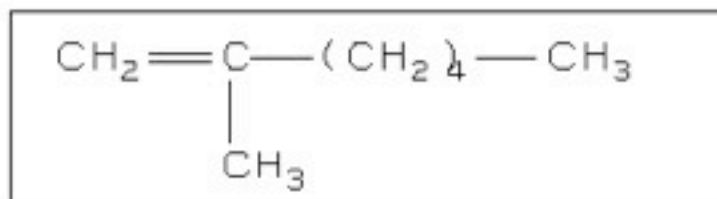


C(sp²)-H伸縮振動

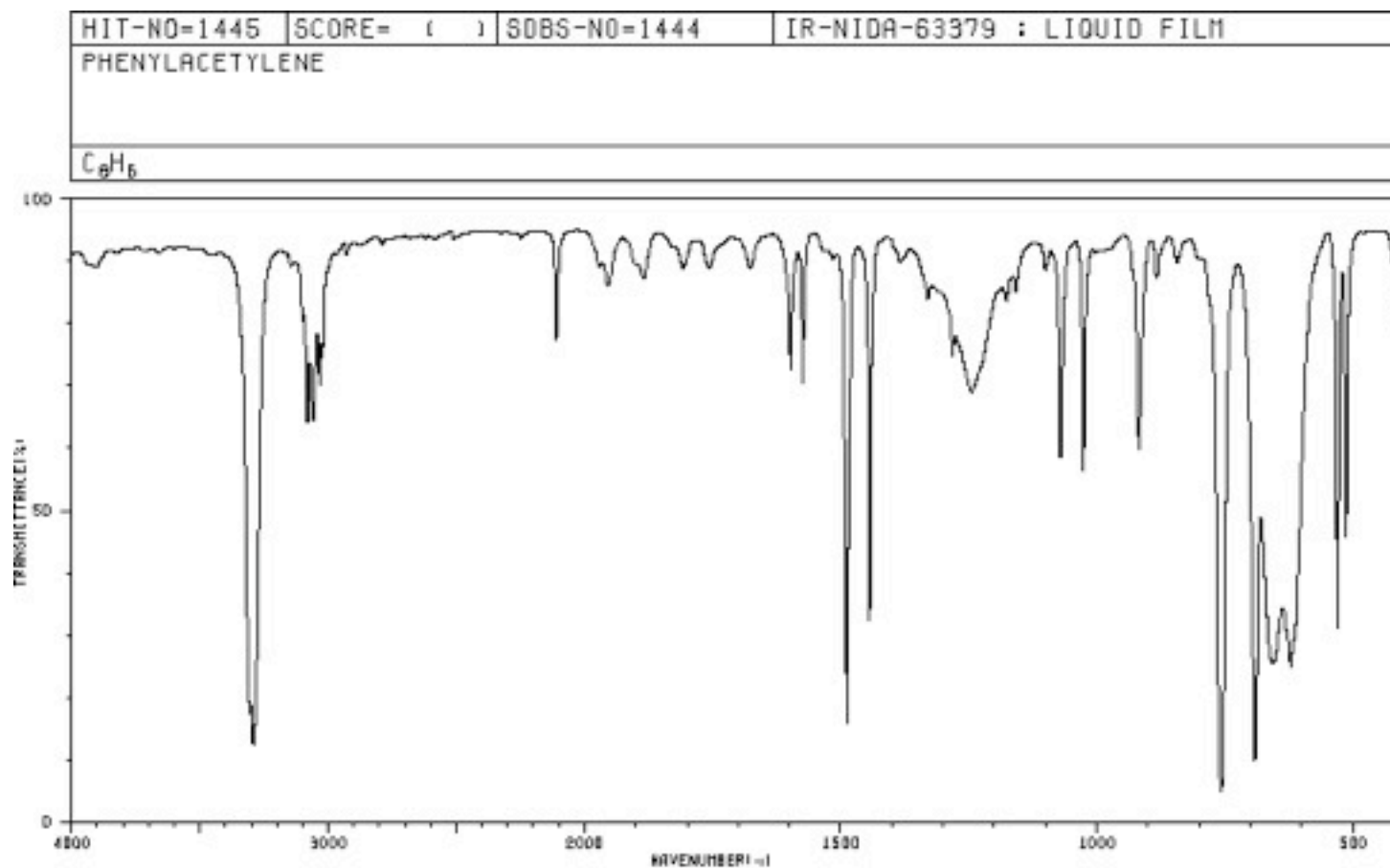
HIT-NO=3282 SCORE= () SDBS-NO=6239 IR-NIDA-10670 ; LIQUID FILM
2-METHYL-1-HEPTENE
C₈H₁₆



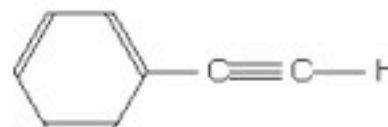
3076	37	1661	29	1108	77
2960	7	1458	27	963	81
2930	4	1375	37	886	9
2874	14	1341	79	769	81
2861	12	1294	81	726	68
2729	77	1278	79	546	74
1780	81	1217	81		



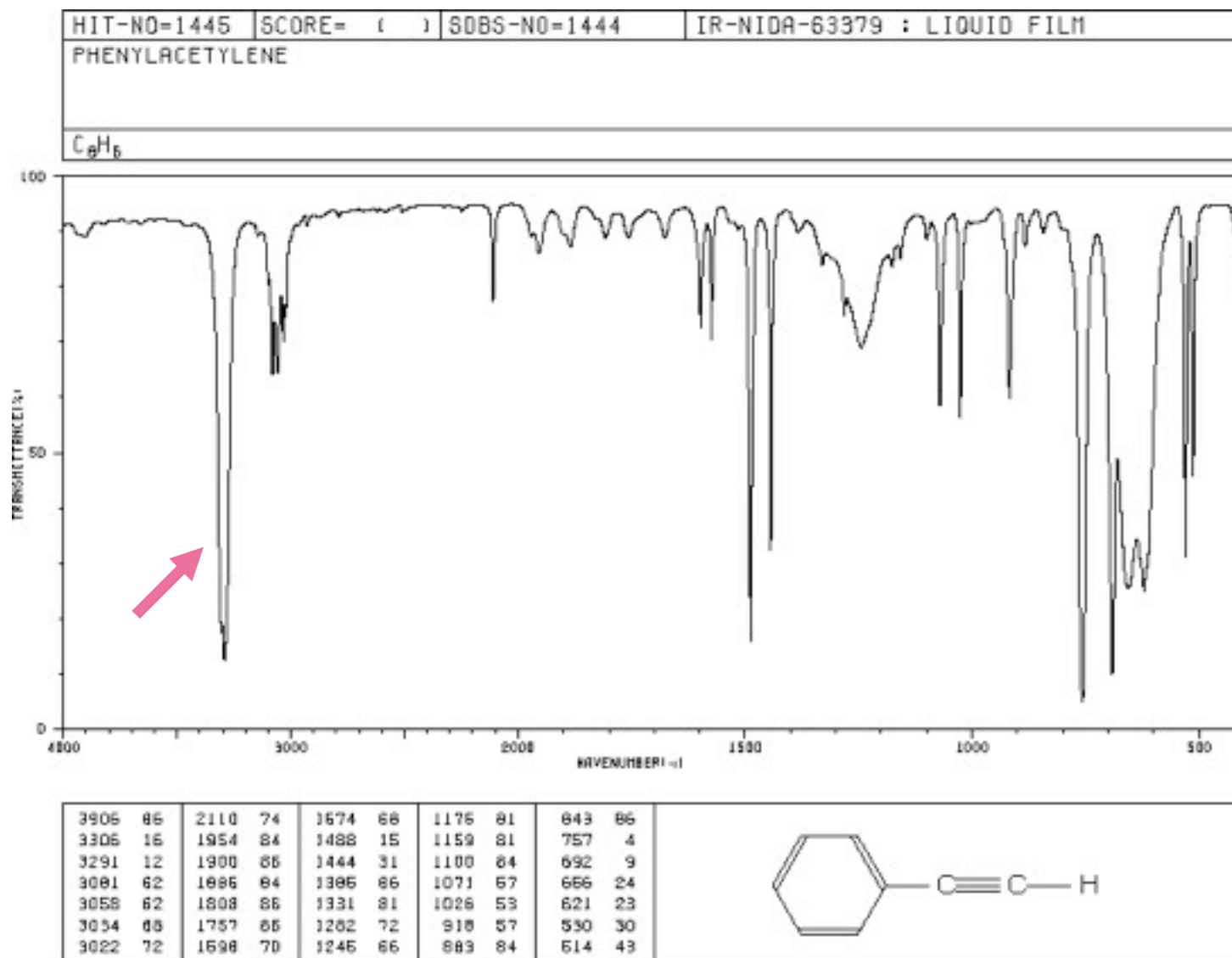
C(sp)-H伸縮振動



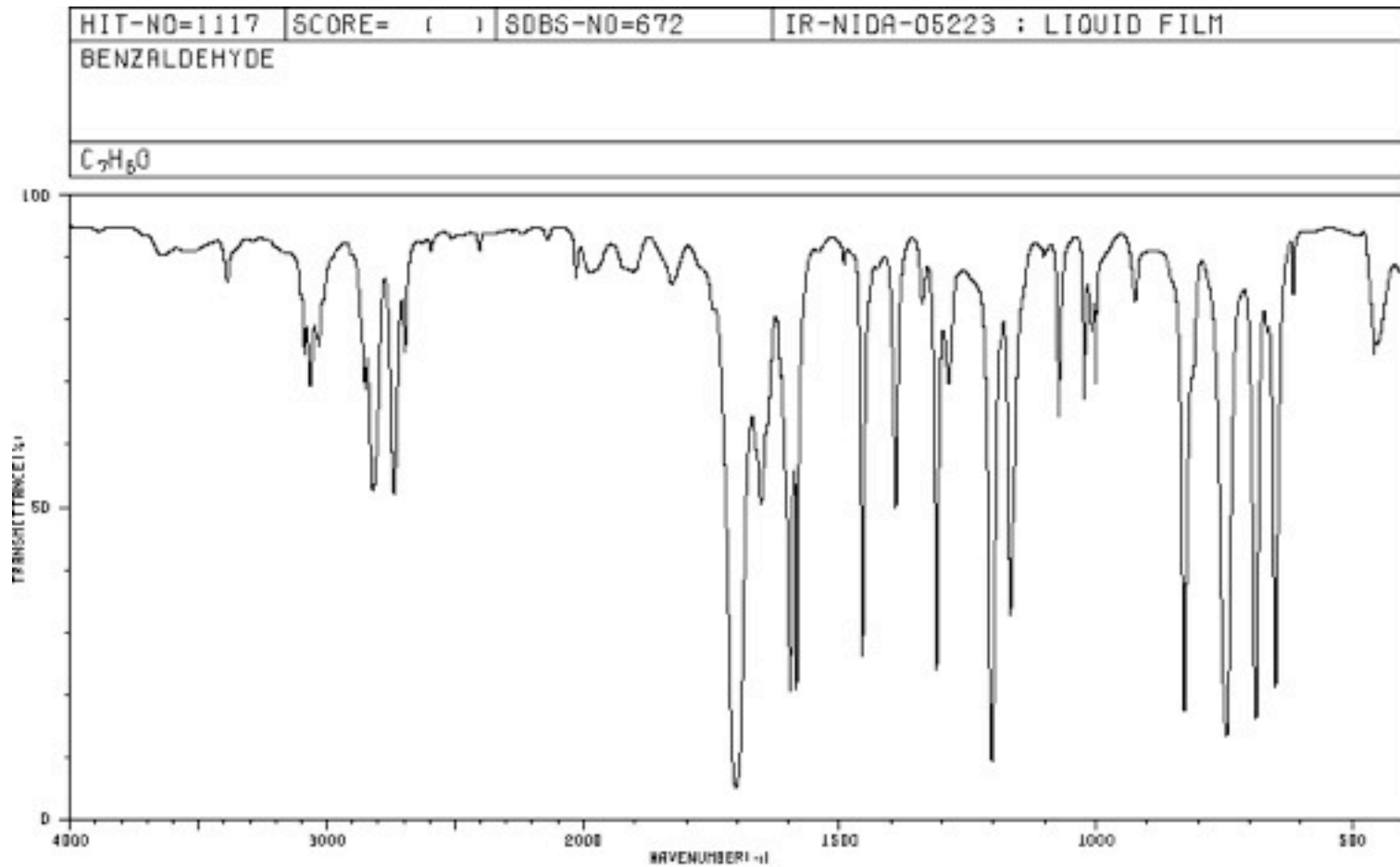
3906	86	2110	74	1674	68	1176	81	843	86
3306	16	1954	84	1488	15	1159	81	757	4
3291	12	1900	86	1444	31	1100	84	692	9
3081	62	1896	84	1386	86	1071	67	666	24
3058	62	1808	86	1331	81	1026	53	621	23
3034	68	1757	86	1262	72	918	57	530	30
3022	72	1698	70	1246	66	883	84	514	43



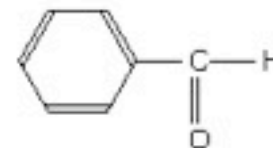
C(sp)-H伸縮振動



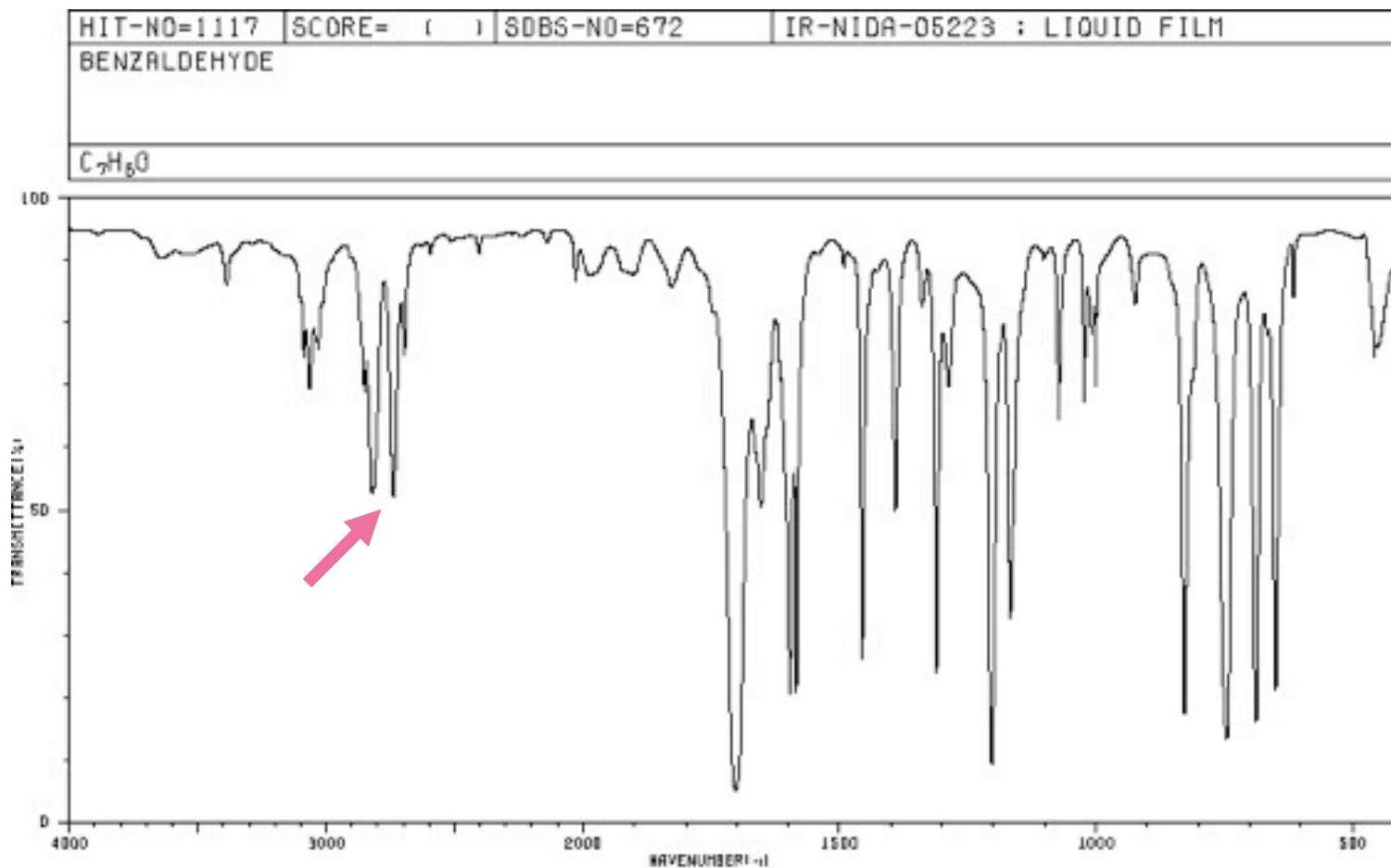
C(sp²)-H伸縮振動 (ホルミル基)



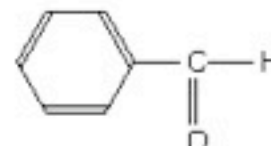
3086	72	1981	84	1697	20	1204	8	828	16
3065	66	1916	84	1584	20	1168	31	746	13
3031	72	1909	84	1456	25	1073	62	668	15
2860	66	1901	84	1391	47	1023	64	667	74
2820	50	1828	81	1339	79	1008	74	650	20
2736	50	1703	4	1311	23	1001	66	615	61
2696	72	1654	49	1288	68	924	79	457	72



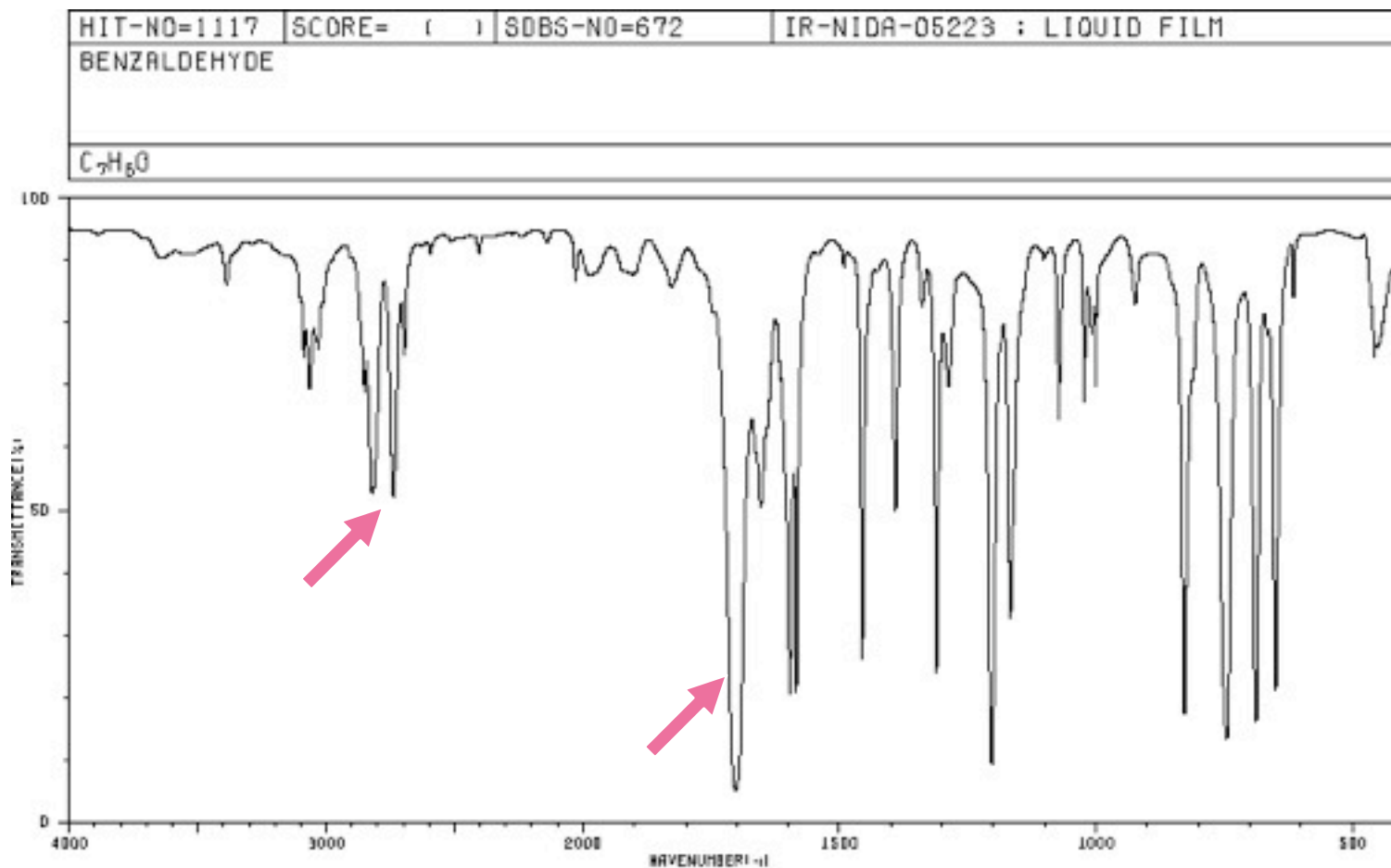
C(sp²)-H伸縮振動 (ホルミル基)



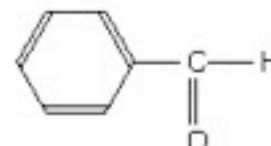
3086	72	1981	84	1697	20	1204	8	828	16
3065	66	1916	84	1584	20	1168	31	746	13
3031	72	1909	84	1456	25	1073	62	688	15
2860	66	1901	84	1391	47	1023	64	667	74
2820	50	1828	81	1339	79	1008	74	650	20
2736	50	1703	4	1311	23	1001	66	615	61
2696	72	1664	40	1288	68	924	70	467	72



C(sp²)-H伸縮振動 (ホルミル基)

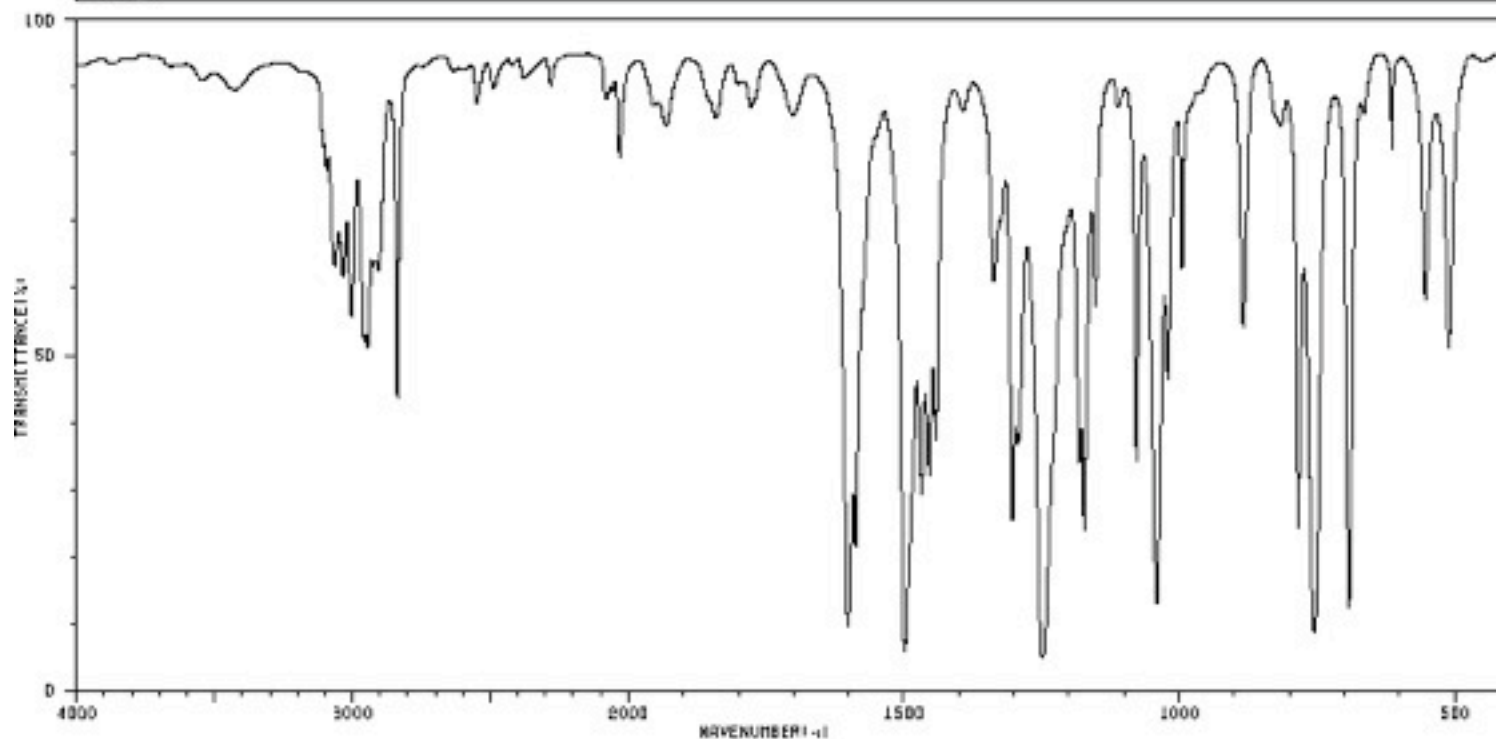


3086	72	1981	84	1697	20	1204	8	828	16
3065	66	1916	84	1584	20	1168	31	746	13
3031	72	1909	84	1456	25	1073	62	688	15
2860	66	1901	84	1391	47	1023	64	667	74
2820	50	1828	81	1339	79	1008	74	650	20
2736	50	1703	4	1311	23	1001	66	615	61
2696	72	1664	40	1288	68	924	70	467	72

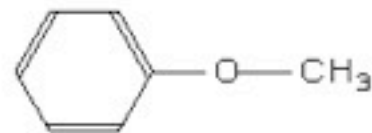


C(sp³)-H伸縮振動 (エーテルのα位)

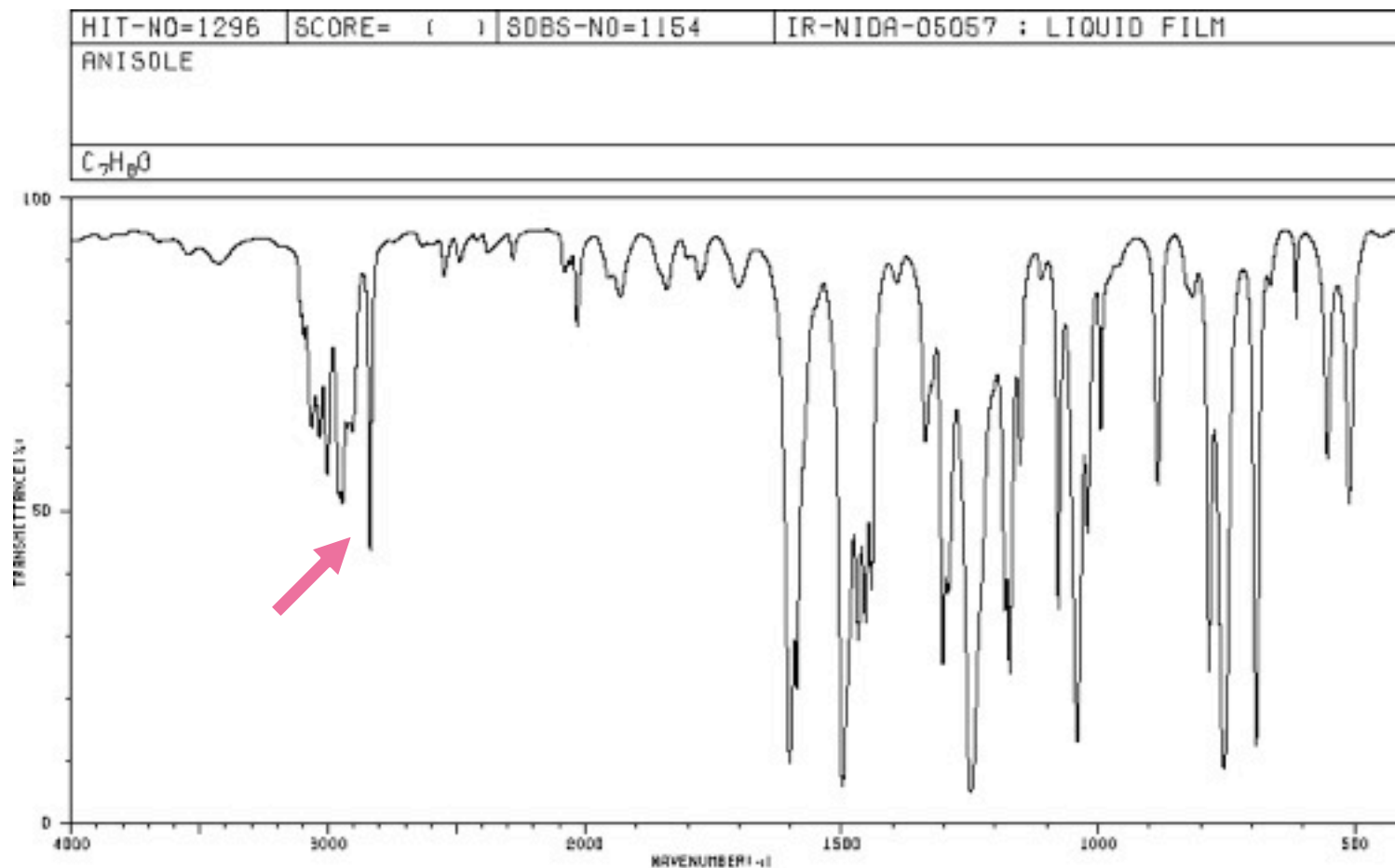
HIT-NO=1296	SCORE= ()	S0BS-NO=1154	IR-NIDA-05057 ; LIQUID FILM
ANISOLE			
C ₇ H ₈ O			



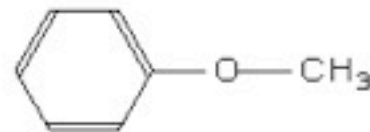
3094	74	2906	60	1468	27	1182	32	884	52
3063	80	2836	42	1454	31	1173	23	784	23
3033	58	2031	77	1442	36	1153	55	755	8
3003	63	1702	81	1337	68	1078	39	692	12
2957	50	1601	9	1303	24	1041	12	614	77
2945	49	1588	20	1293	35	1021	44	553	57
2926	60	1498	5	1248	4	995	60	511	49



C(sp³)-H伸縮振動 (エーテルのα位)

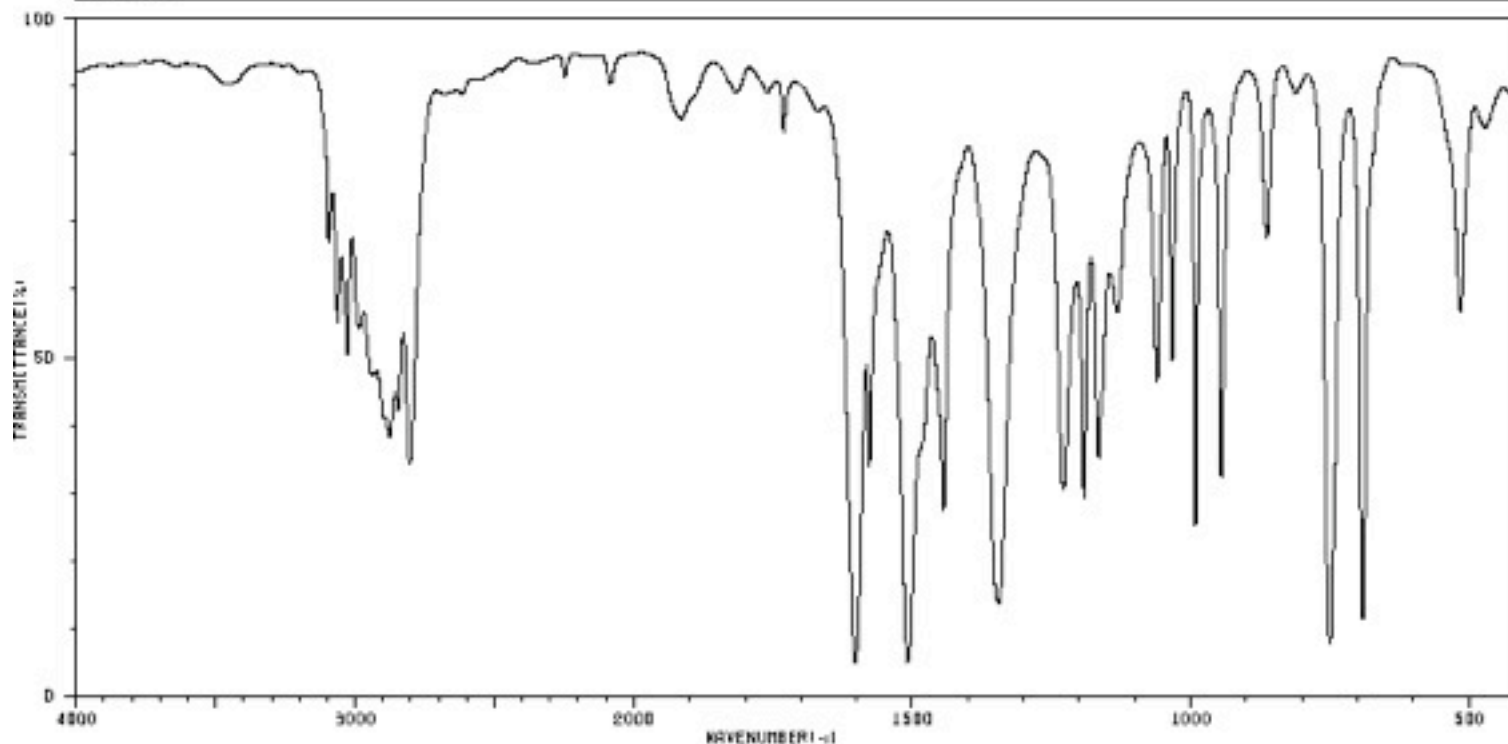


3094	74	2906	60	1468	27	1182	32	684	52
3063	60	2836	42	1454	31	1173	29	784	23
3033	58	2031	77	1442	36	1153	55	755	8
3009	63	1702	81	1337	68	1078	39	692	12
2957	50	1601	9	1303	24	1041	12	614	77
2945	49	1588	20	1293	35	1021	44	553	57
2926	60	1498	5	1248	4	996	60	611	49

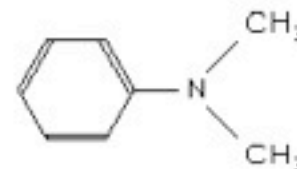


C(sp³)-H伸縮振動 (アミンのα位)

HIT-NO=1600	SCORE= ()	SDBS-NO=1852	IR-NIDA-05008 : LIQUID FILM
N,N-DIMETHYLANILINE			
C ₈ H ₁₁ N			

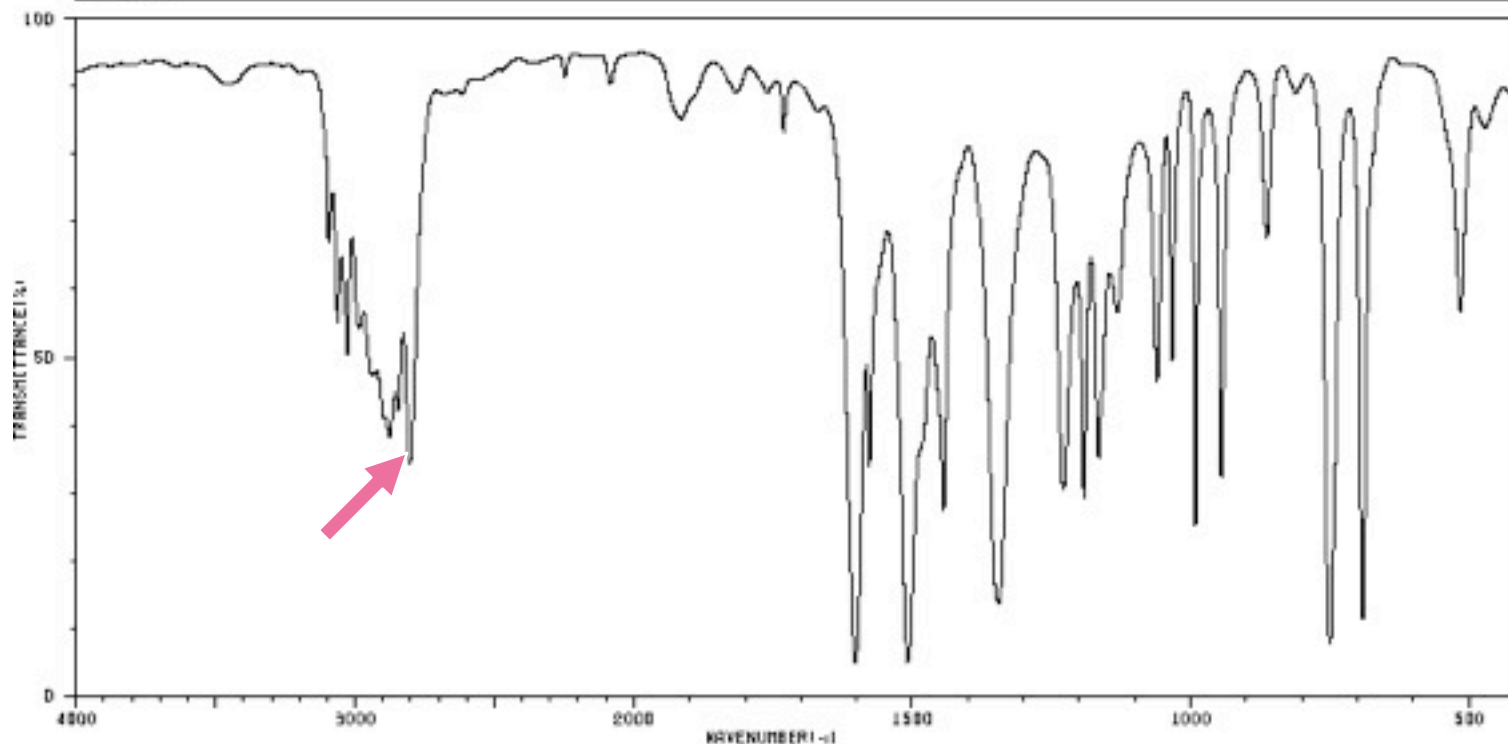


3094	64	2804	39	1609	4	1051	44	760	7
3063	53	1915	81	1444	26	1033	47	692	10
3027	49	1818	86	1345	15	981	25	516	55
2984	62	1760	86	1229	29	981	74	473	81
2893	39	1731	78	1192	27	945	31		
2875	36	1602	4	1167	34	854	64		
2846	41	1577	32	1131	66	813	86		



C(sp³)-H伸縮振動 (アミンのα位)

HIT-NO=1600	SCORE= ()	SDBS-NO=1852	IR-NIDA-05008 : LIQUID FILM
N,N-DIMETHYLANILINE			
C ₈ H ₁₁ N			



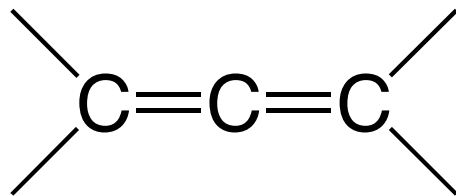
3094	64	2804	39	1609	4	1051	44	760	7
3063	53	1915	81	1444	26	1033	47	692	10
3027	49	1818	86	1345	15	981	25	516	55
2984	62	1760	86	1229	29	981	74	473	81
2893	39	1731	78	1192	27	945	31		
2875	36	1602	4	1167	34	854	64		
2846	41	1577	32	1131	66	813	86		

2500 cm⁻¹ ~ 1900 cm⁻¹

(不毛な領域)



対称分子は赤外不活性

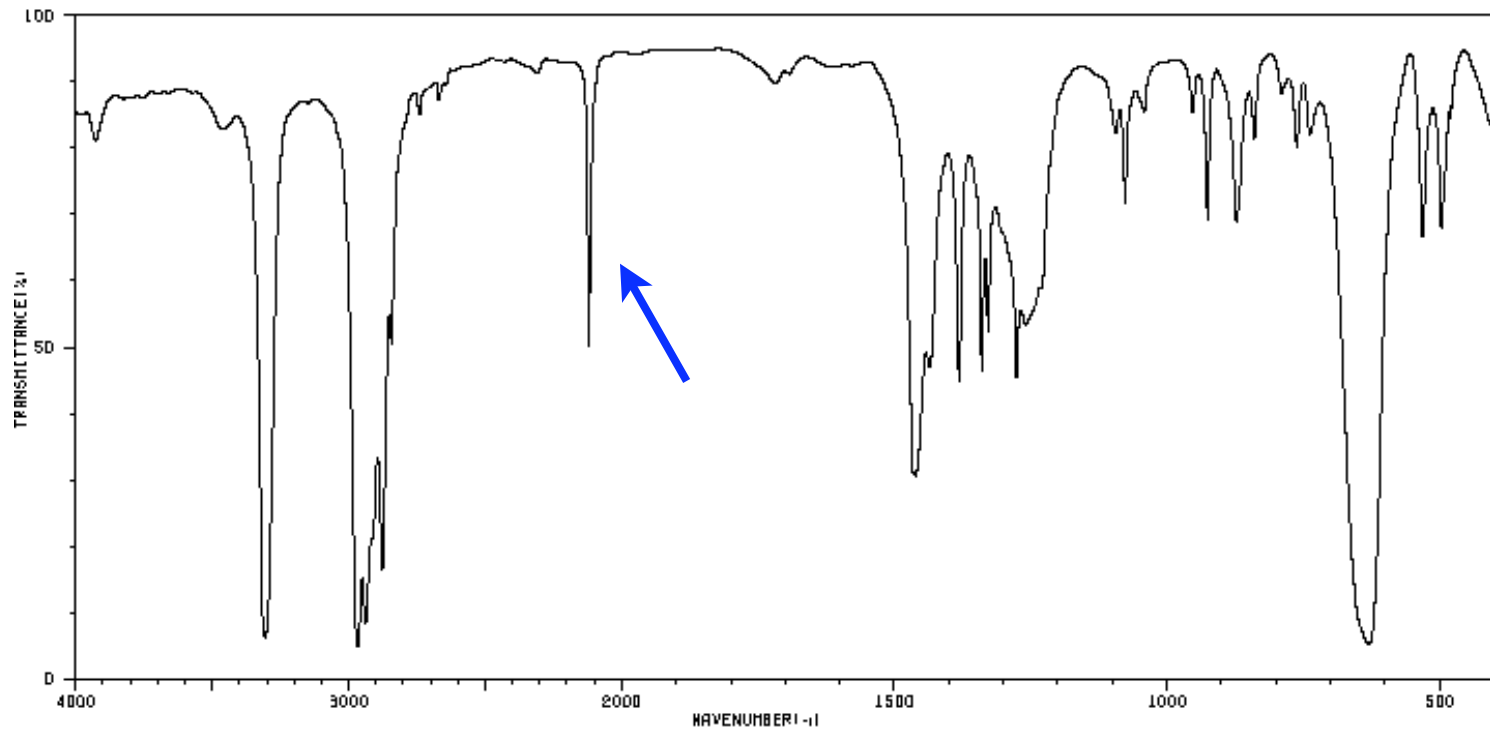


累積二重結合



C≡C 伸縮振動 (1)

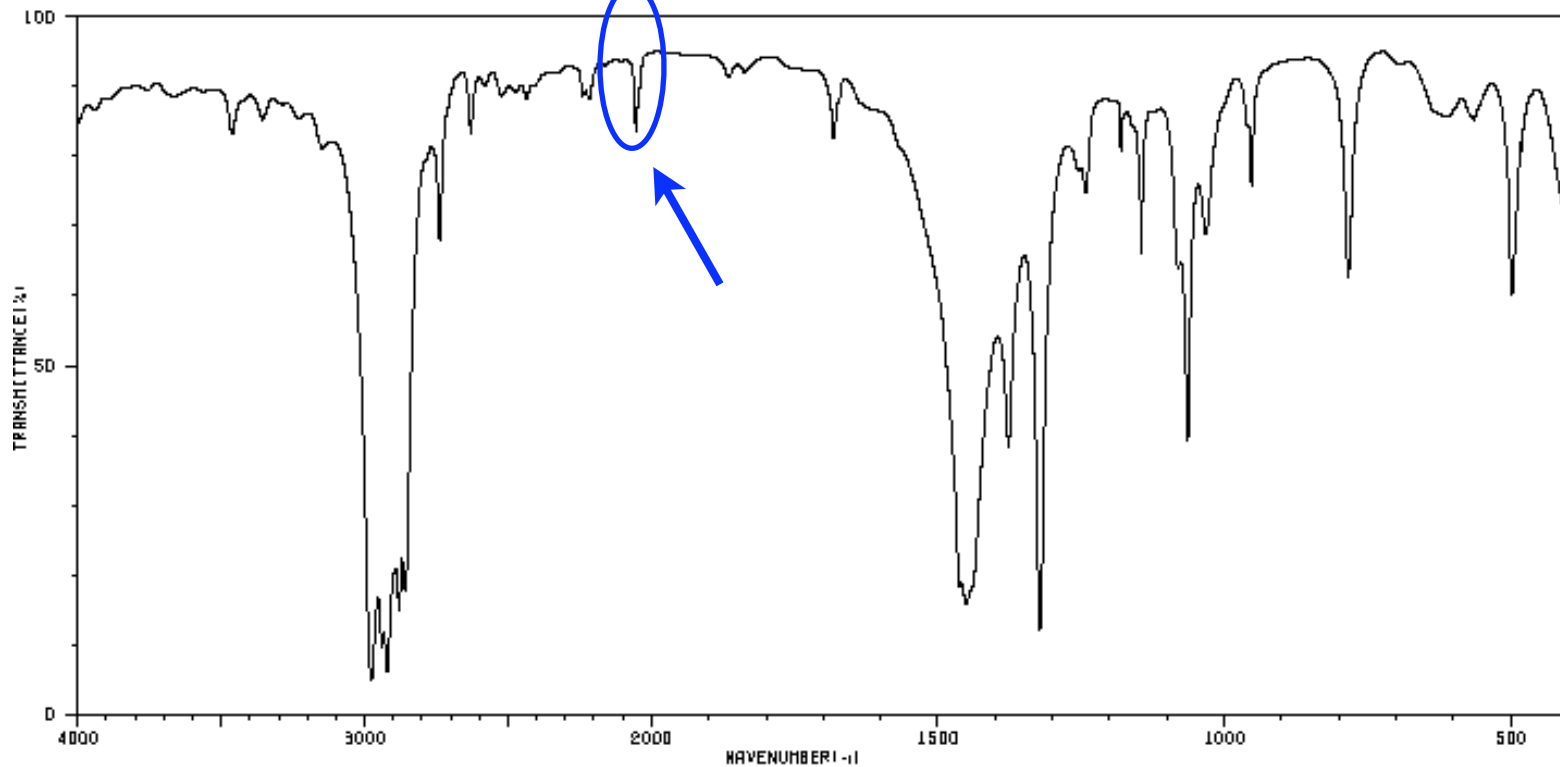
HIT-NO=2943	SCORE= ()	SDBS-NO=5386	IR-NIDA-13676 : LIQUID FILM
1-PENTYNE			
C ₅ H ₈			



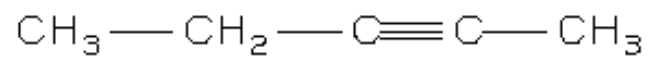
3928	79	2741	81	1381	43	1041	81	739	79	$\text{CH}_3 - (\text{CH}_2)_2 - \text{C} \equiv \text{CH}$
3457	79	2670	84	1340	44	954	81	630	5	
3307	6	2120	47	1328	50	926	66	532	64	
2968	4	1718	86	1276	43	872	66	497	66	
2938	7	1466	29	1259	52	840	79	481	81	
2876	16	1460	29	1095	79	791	84			
2843	49	1436	44	1077	68	762	77			

C≡C 伸縮振動 (2)

HIT-NO=2944 SCORE= () SDBS-NO=5387 IR-NIDA-13678 : LIQUID FILM
 2-PENTYNE
 C_5H_8

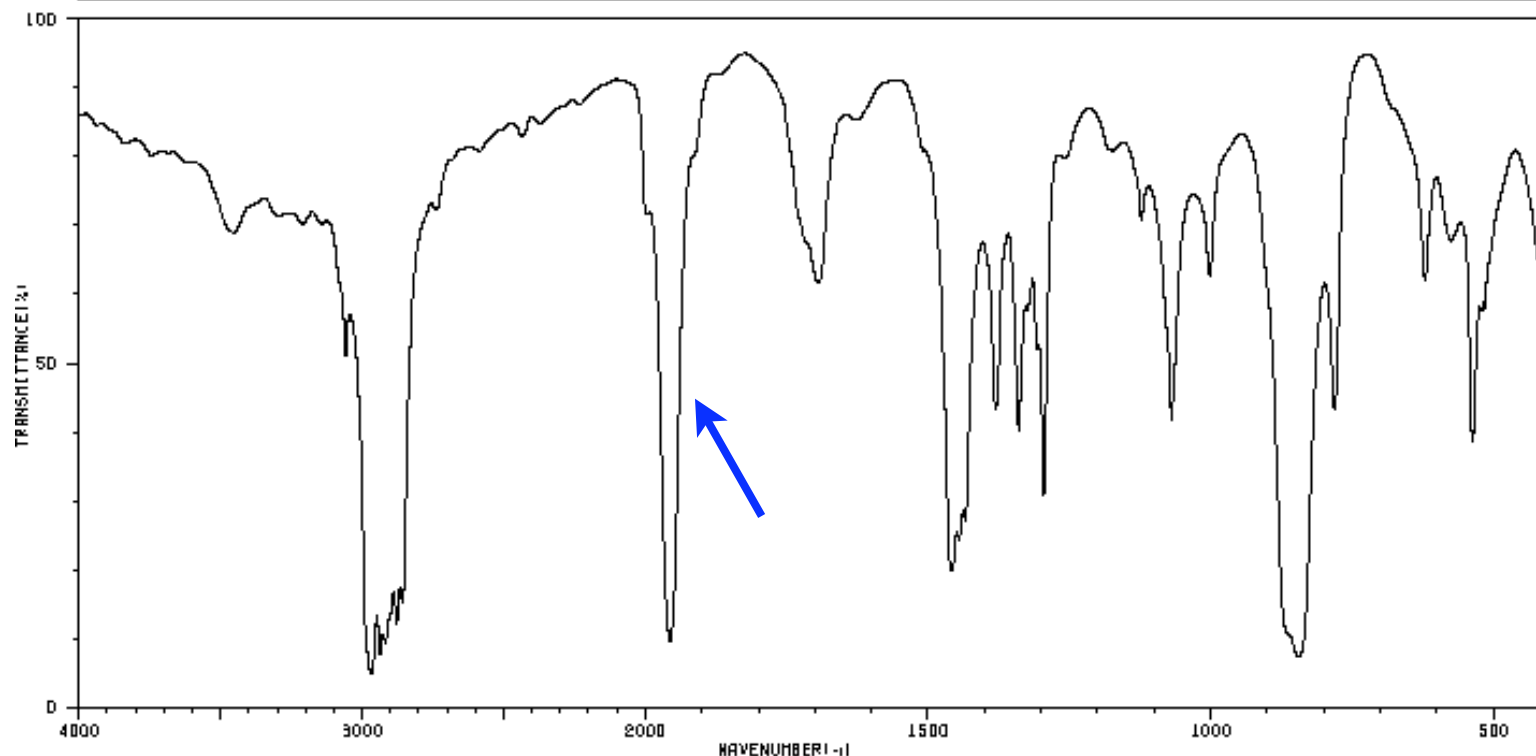


3669	84	2860	17	1682	79	1181	77	963	72
3463	79	2739	66	1463	17	1158	81	784	60
3354	81	2629	79	1451	15	1145	64	619	61
2976	4	2436	84	1377	37	1081	62	613	81
2940	9	2239	84	1322	11	1064	37	583	81
2922	6	2218	84	1256	74	1032	66	499	57
2879	14	2063	81	1243	72	960	81	481	77



C=C伸縮振動 (累積二重結合)

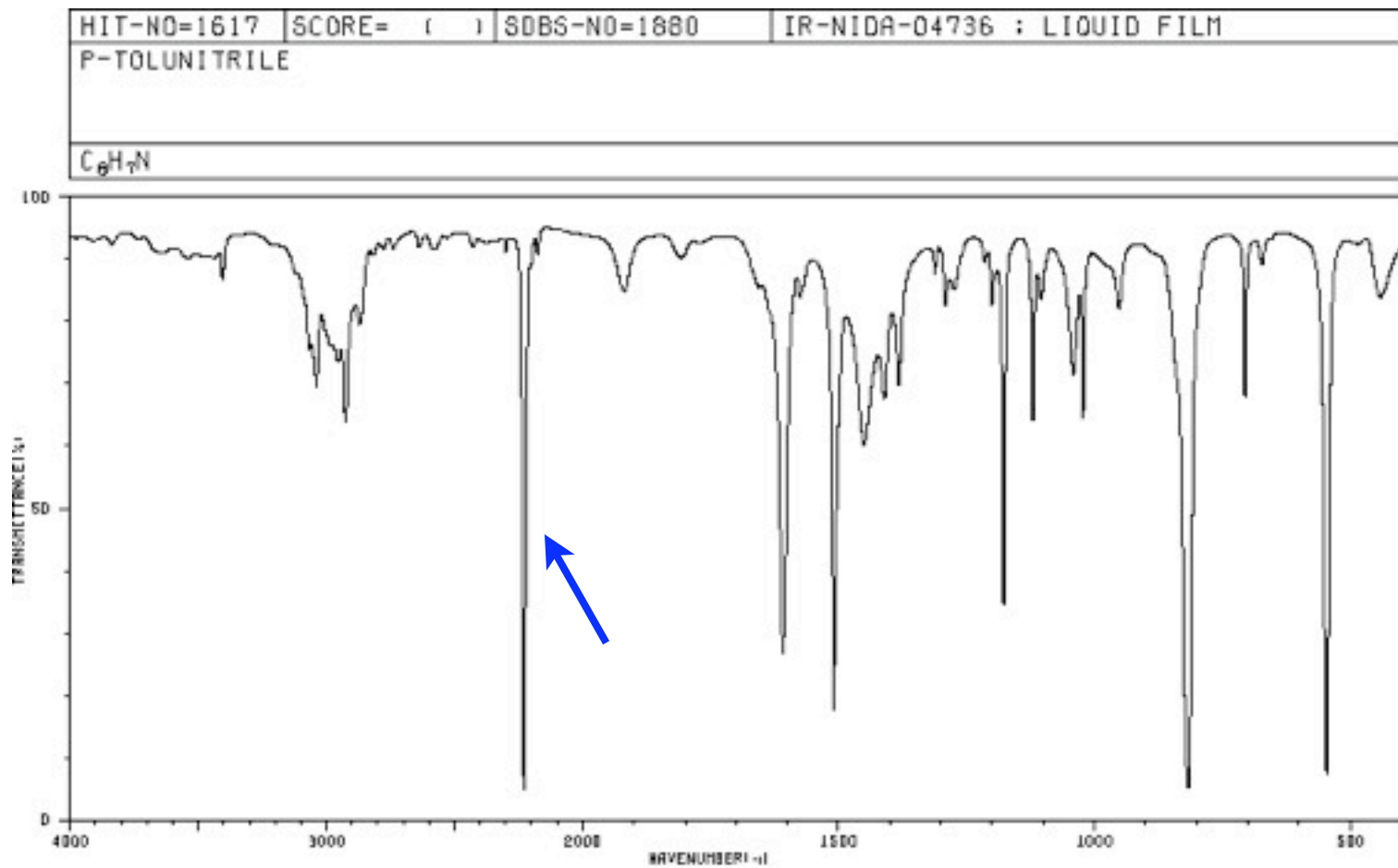
HIT-NO=2942	SCORE= ()	SDBS-NO=5385	IR-NIDA-13610 : LIQUID FILM
1,2-PENTADIENE			
C ₅ H ₈			



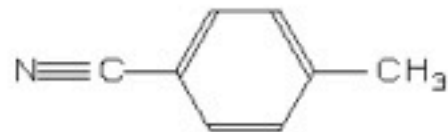
3464	66	2869	14	1434	26	1070	39	538	37
3210	68	2434	79	1381	42	1006	64	521	55
3059	49	2370	81	1340	38	1001	60		
2968	4	1966	9	1308	50	844	7		
2936	7	1693	58	1296	29	781	42		
2917	9	1458	19	1174	77	622	60		
2877	12	1446	29	1123	68	576	66		

$$\text{CH}_2=\text{C}=\text{CH}-\text{CH}_2-\text{CH}_3$$

C≡N 伸縮振動

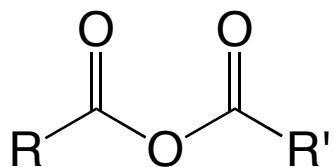


3404	84	2201	86	1411	64	1190	84	817	6
3068	72	1919	81	1383	68	1178	39	706	66
3039	86	1609	26	1312	84	1120	62	673	86
2966	70	1576	81	1291	79	1104	78	546	7
2926	62	1568	81	1274	81	1041	68	441	81
2869	77	1509	17	1215	86	1022	62		
2229	4	1460	68	1201	79	962	79		

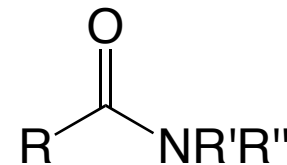
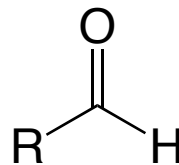
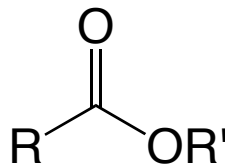
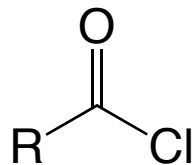
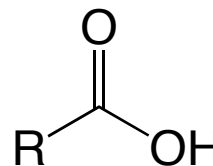
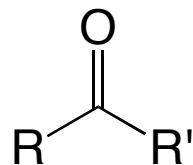


1900 cm^{-1} ~ 1500 cm^{-1}

(**C=O**, C=C, C=N 伸縮、NH変角)

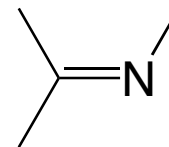


(2個の吸収)

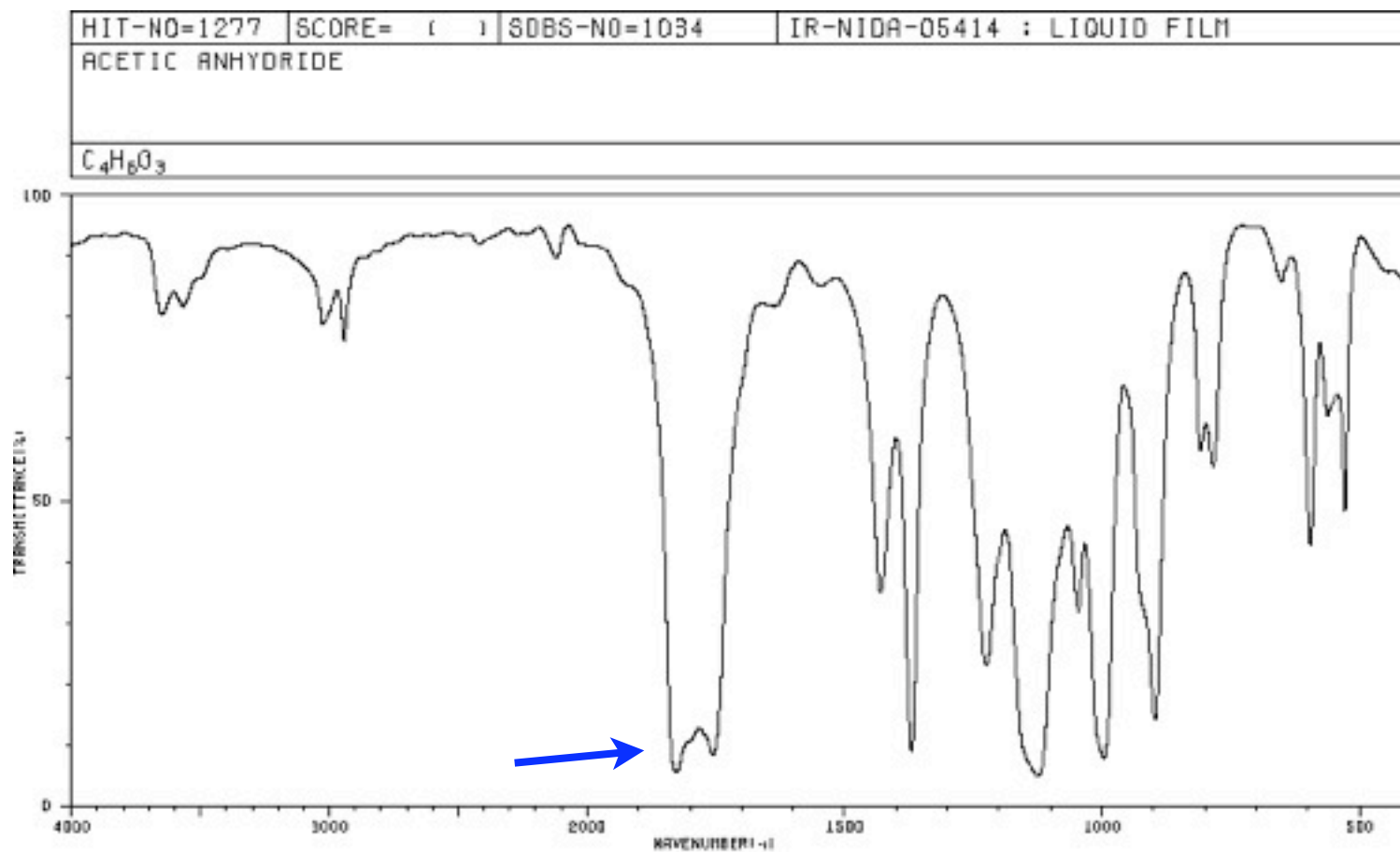


1800

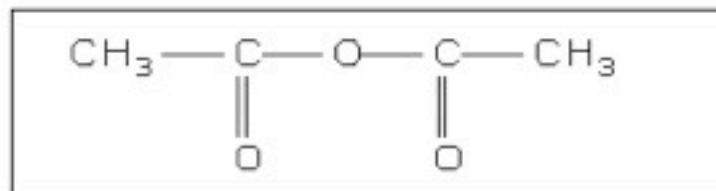
1700



C=O伸縮振動 (酸無水物)

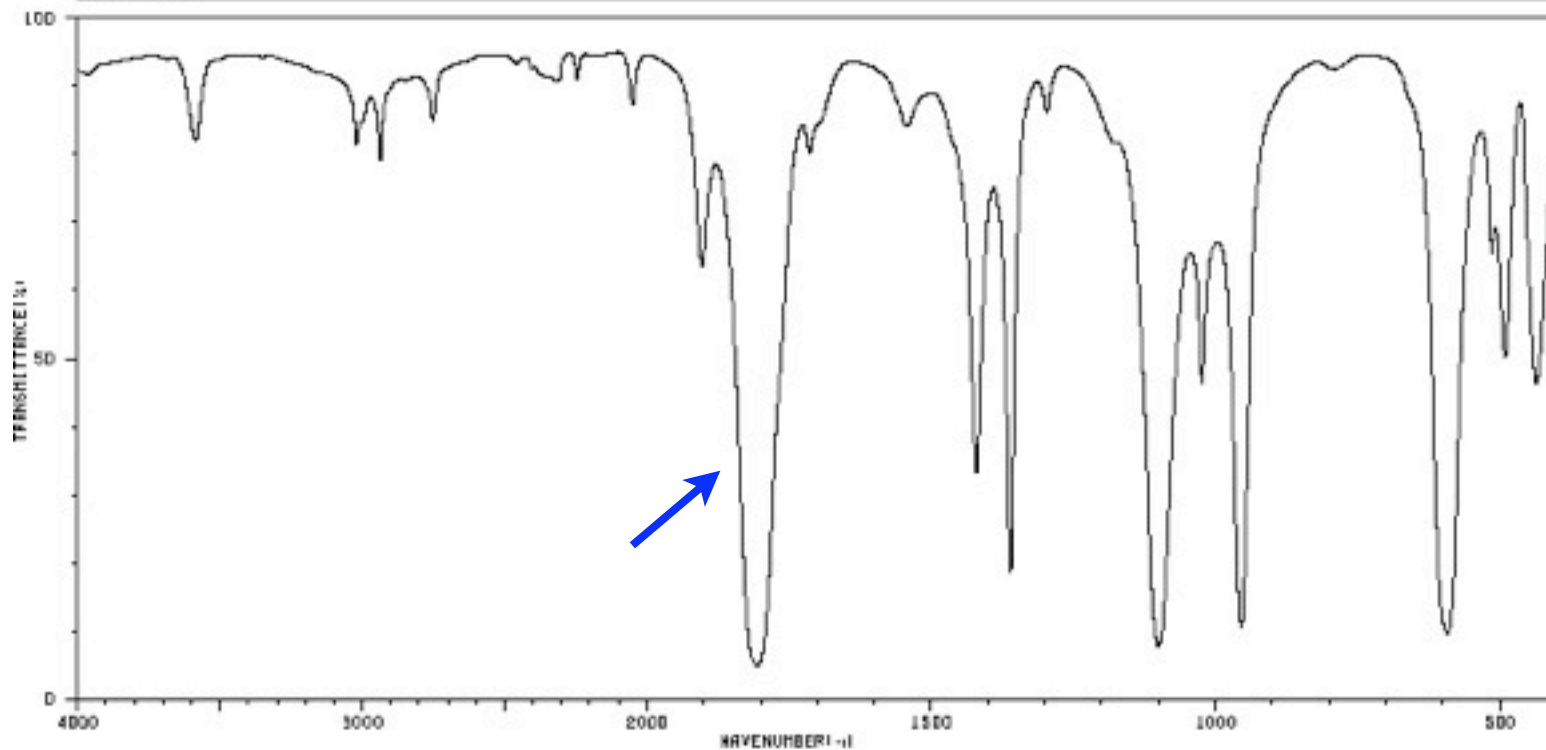


3660	77	1647	81	997	7	563	62
3567	79	1542	81	897	13	543	64
3025	77	1430	35	809	55	529	46
2942	72	1370	8	799	60		
2119	86	1226	22	784	53		
1827	5	1124	4	651	81		
1765	8	1046	30	606	41		

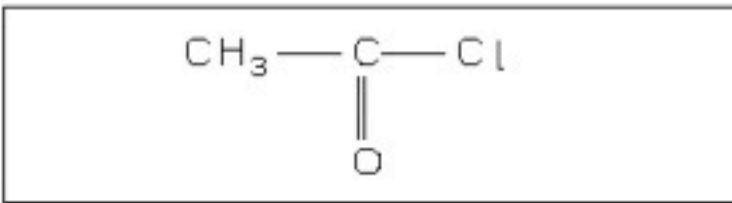


C=O伸縮振動 (酸塩化物)

HIT-NO=1359 SCORE= () SDBS-NO=1278 IR-NIDA-04097 ; LIQUID FILM
ACETYL CHLORIDE
C₂H₃ClO

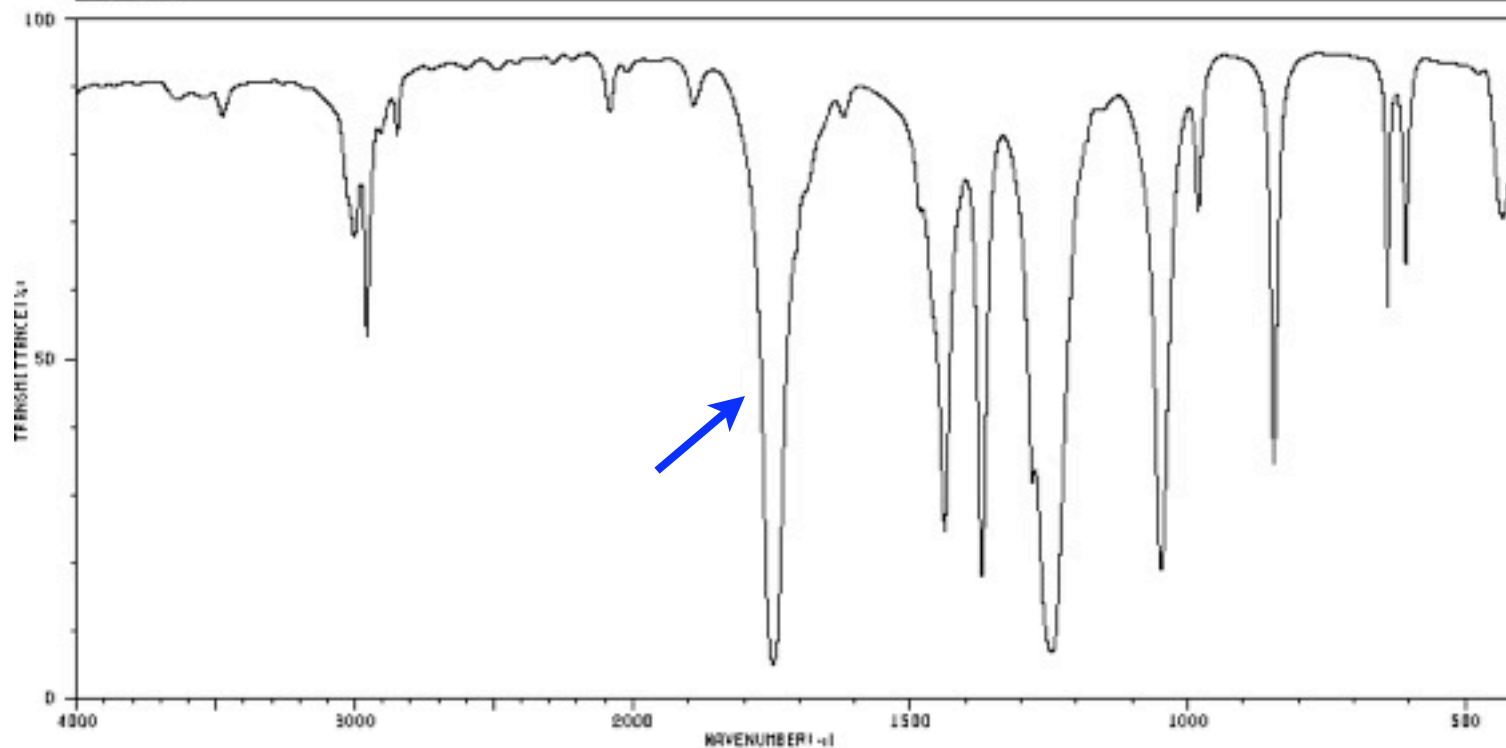


3586	79	1806	4	1024	44
3020	79	1714	77	955	10
2997	81	1542	81	593	9
2937	77	1421	32	616	62
2751	81	1361	18	491	47
2051	84	1297	84	461	84
1903	60	1100	7	436	44

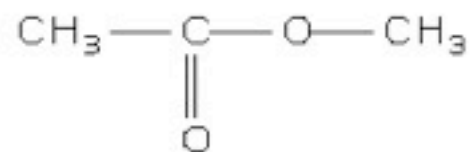


C=O伸縮振動 (エステル)

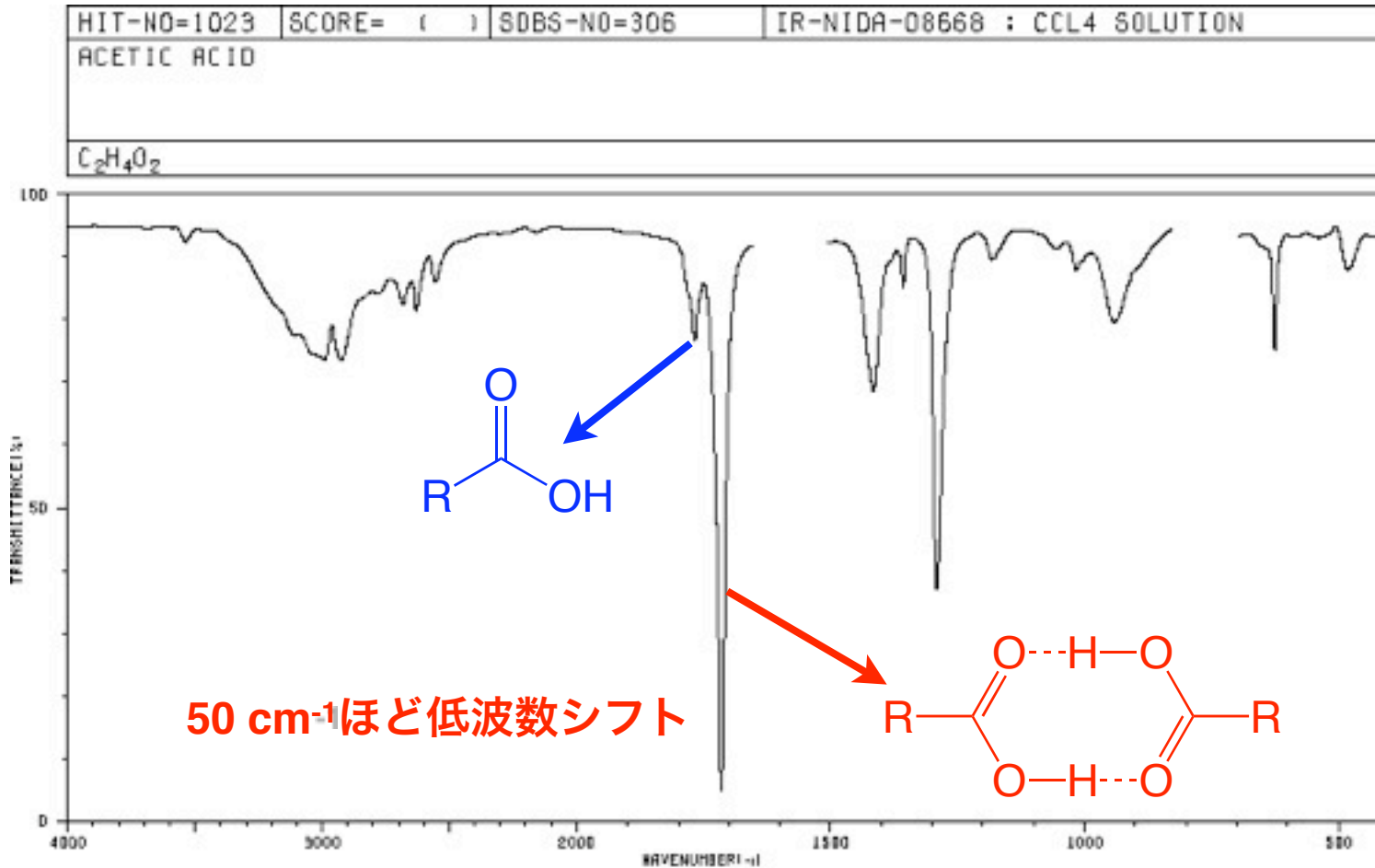
HIT-NO=2024	SCORE= ()	SDBS-NO=2778	IR-NIDA-00511 : LIQUID FILM
METHYL ACETATE			
C ₃ H ₆ O ₂			



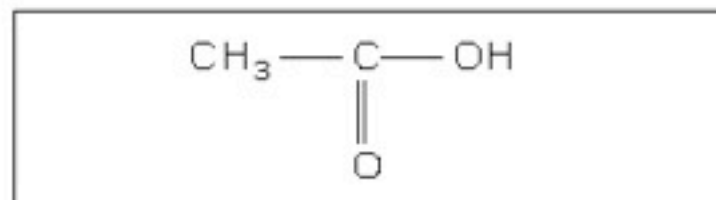
3476	81	1620	81	846	33
3002	66	1438	23	640	55
2957	50	1371	17	608	80
2848	79	1280	30	433	68
2082	84	1246	6		
1890	84	1048	18		
1746	4	981	68		



C=O伸縮振動 (カルボン酸)

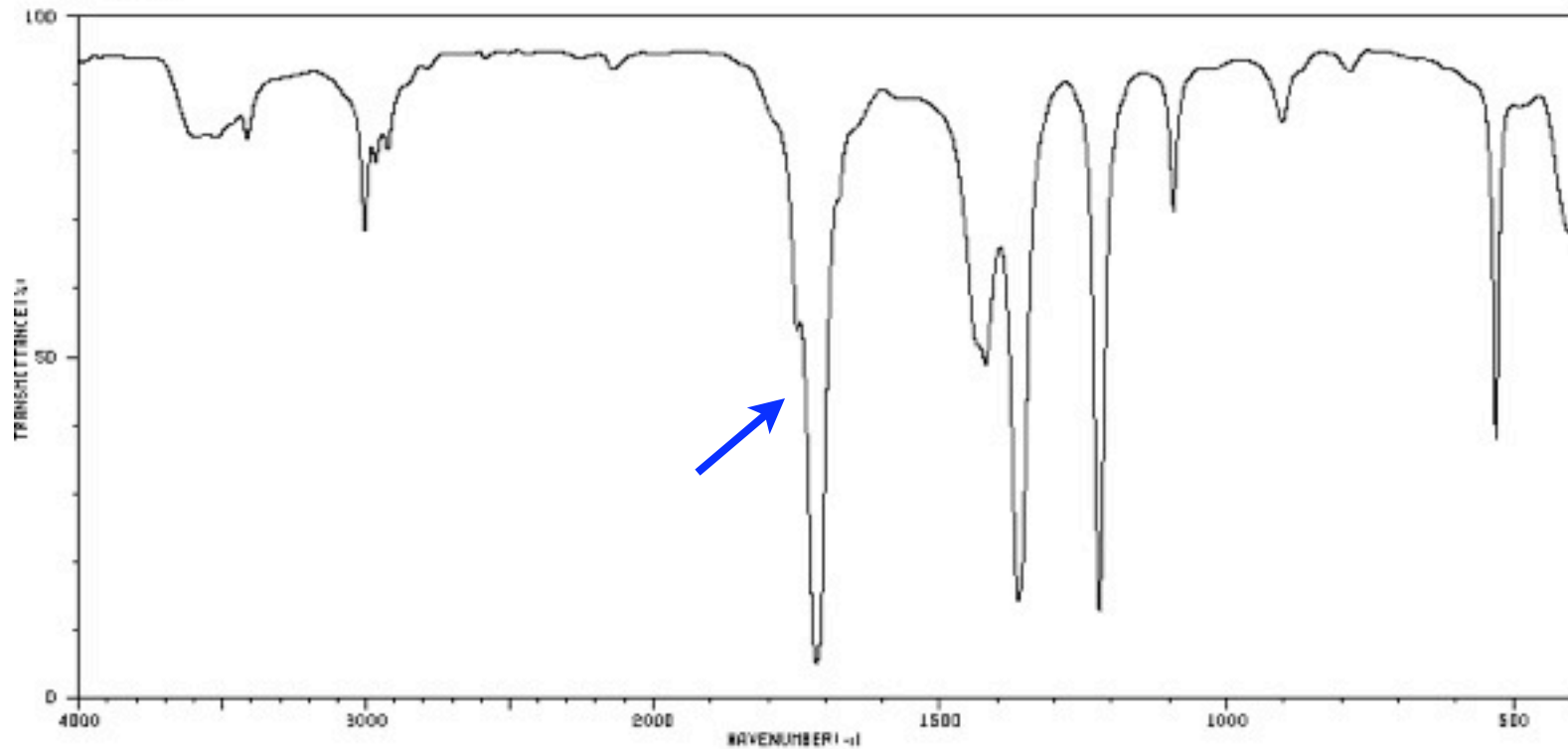


3021	72	2556	81	1018	84
3010	72	1768	74	942	77
3000	70	1715	4	827	72
2989	70	1416	68	482	84
2925	70	1358	81		
2882	79	1292	35		
2630	79	1183	86		

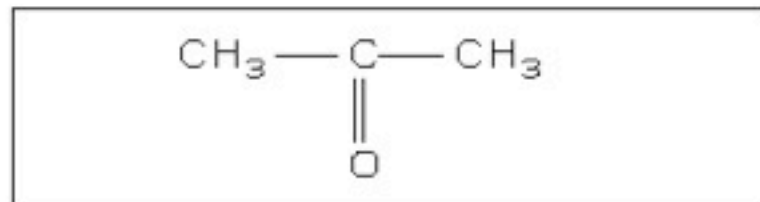


C=O伸縮振動 (ケトン)

HIT-NO-960	SCORE= ()	SDBS-NO-319	IR-NIDA-63533 : LIQUID FILM
ACETONE			
C ₃ H ₆ O			

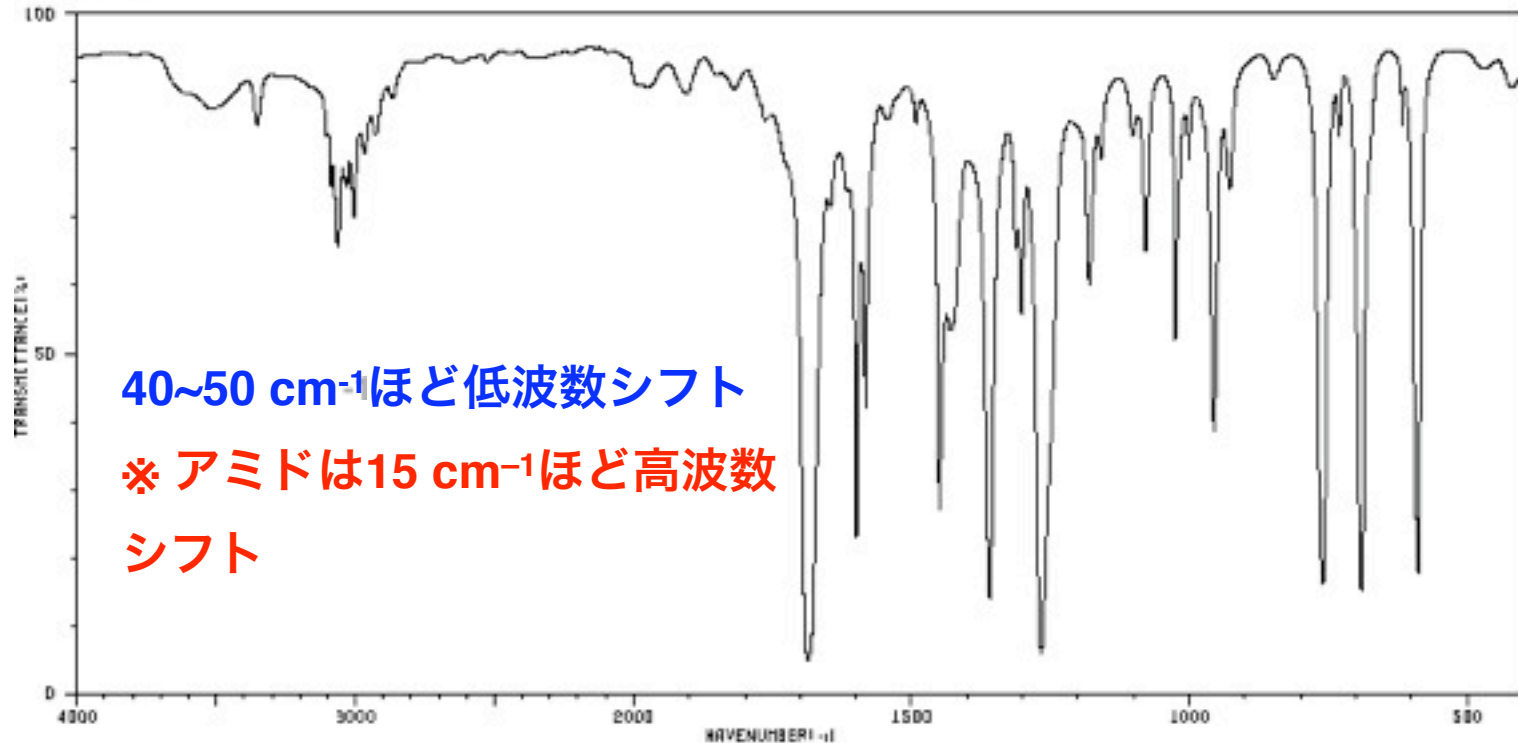


3414	79	1421	47
3005	66	1363	19
2966	74	1223	12
2926	77	1093	68
1749	52	903	81
1715	4	531	56
1434	49		

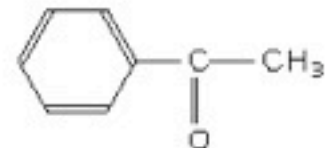


C=O伸縮振動 (共役ケトン)

HIT-NO=1153 SCORE= () SDBS-NO=722 IR-NIDA-05227 : LIQUID FILM
 ACETOPHENONE
 C_8H_8O

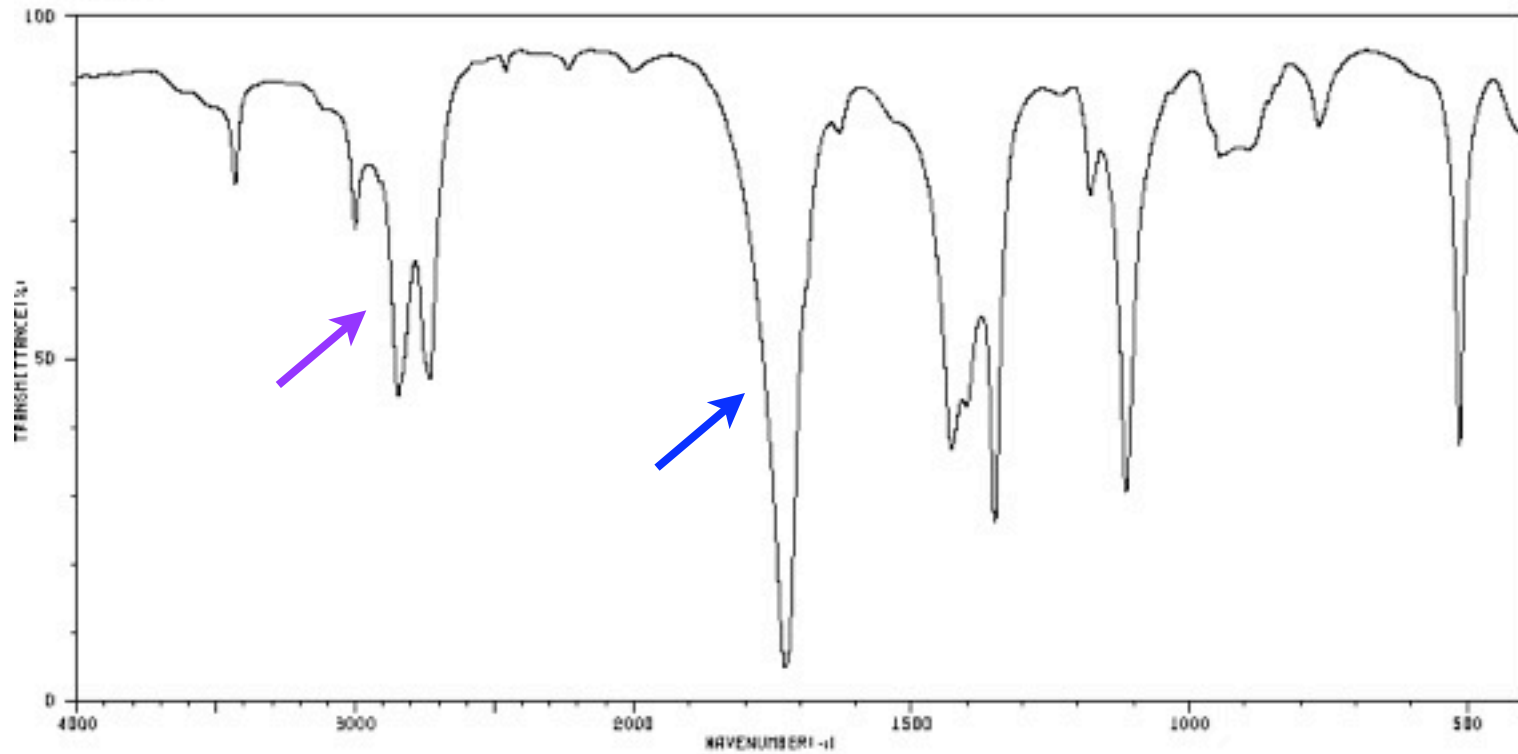


3604	84	2967	77	1646	81	1267	6	966	37
3352	81	2925	79	1492	81	1181	58	928	72
3087	72	2867	84	1450	26	1160	74	761	15
3063	64	1606	4	1430	52	1103	79	731	79
3040	72	1546	68	1360	13	1079	62	691	14
3029	72	1599	21	1313	82	1025	50	618	61
3006	68	1583	41	1303	53	1001	74	598	17

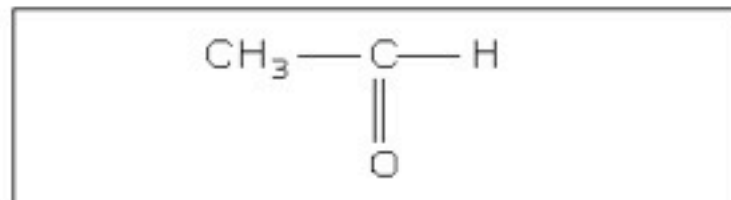


C=O伸縮振動 (アルデヒド)

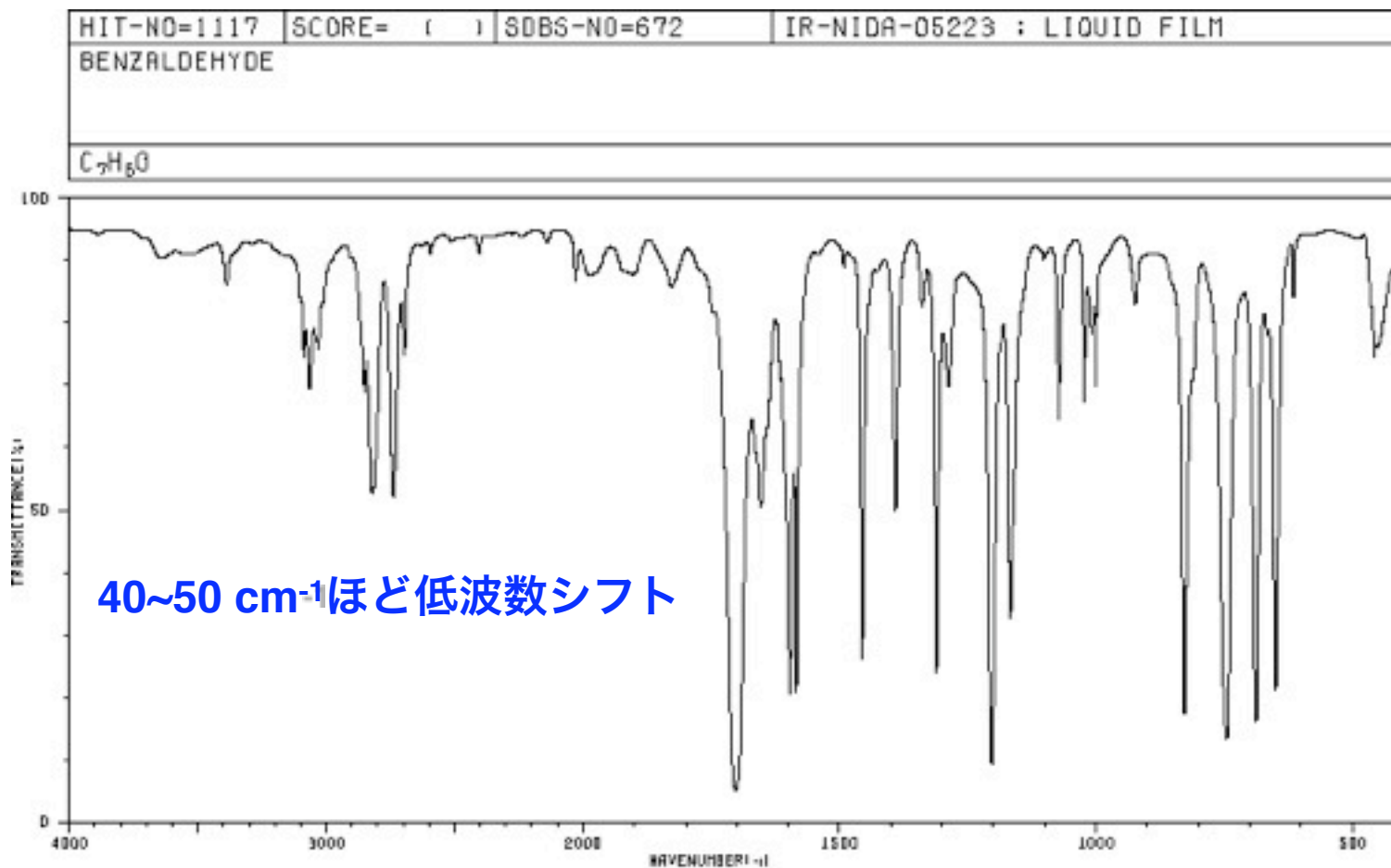
HIT-NO=949	SCORE= ()	SDBS-NO=305	IR-NIDA-40660 : LIQUID FILM
ACETALDEHYDE			
C ₂ H ₄ O			



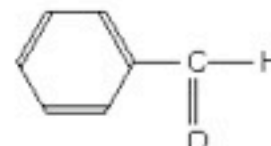
3432	72	1401	41
3001	66	1350	25
2846	42	1179	70
2739	44	1114	29
1727	4	945	77
1629	79	767	61
1429	36	614	36



C=O伸縮振動（共役アルデヒド）

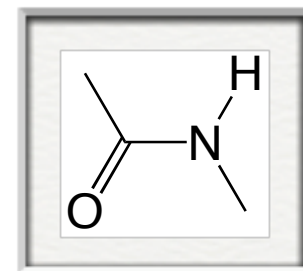
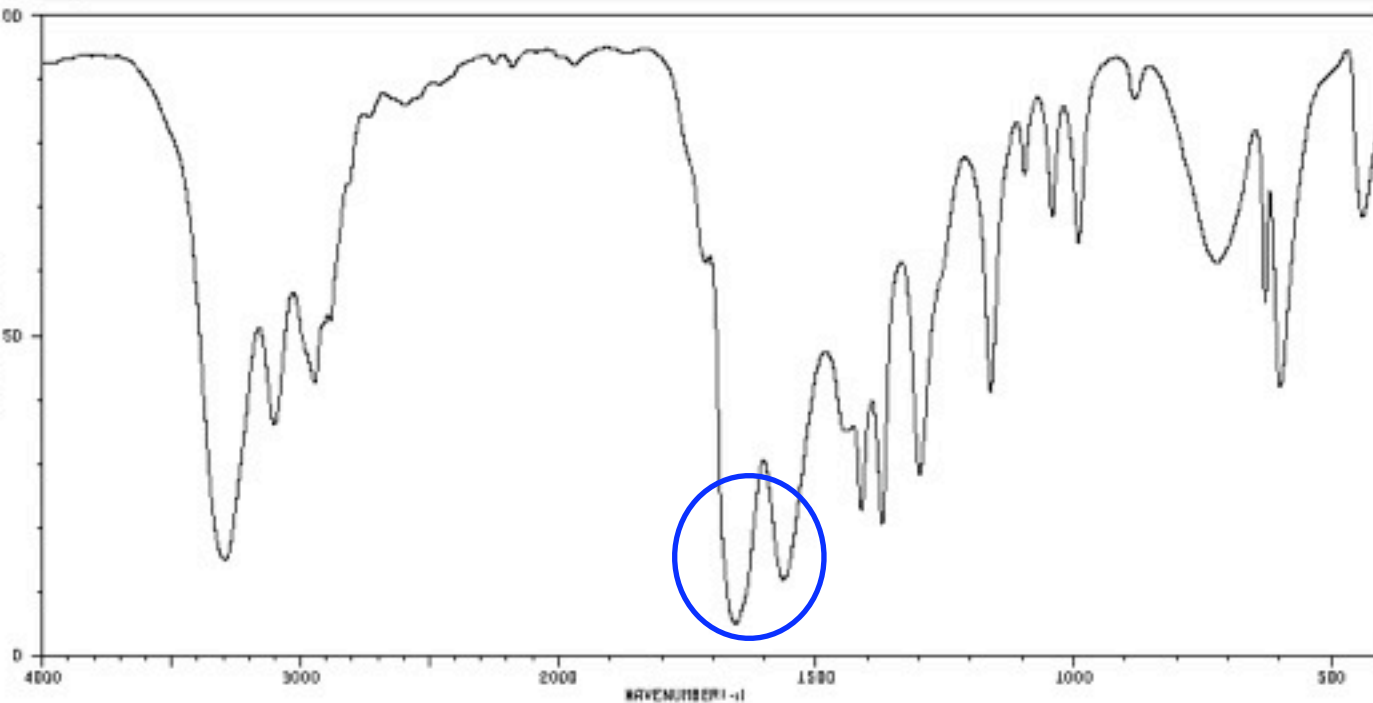


3086	72	1981	84	1697	20	1204	8	828	16
3065	66	1916	84	1584	20	1168	31	746	13
3031	72	1909	84	1456	25	1073	62	688	15
2860	66	1901	84	1391	47	1023	64	667	74
2820	50	1828	81	1339	79	1008	74	650	20
2736	50	1703	4	1311	23	1001	66	615	61
2696	72	1664	40	1288	68	924	70	467	72

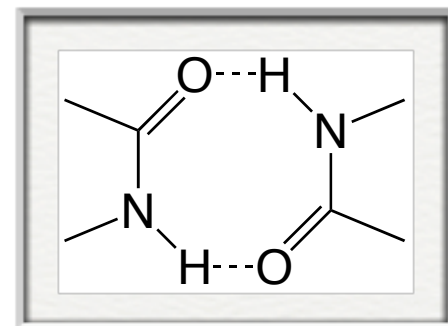


C=O伸縮振動 (アミド)

HIT-NO-2452 SCORE= () SDBS-NO-4002 IR-NIDA-63942 : LIQUID FILM
 N-METHYLACETAMIDE
 C_3H_7NO

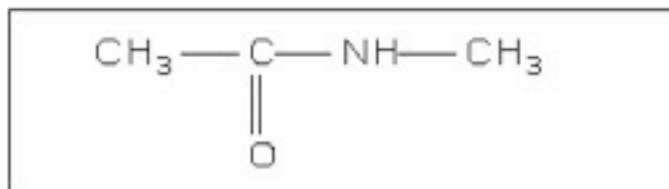


I型



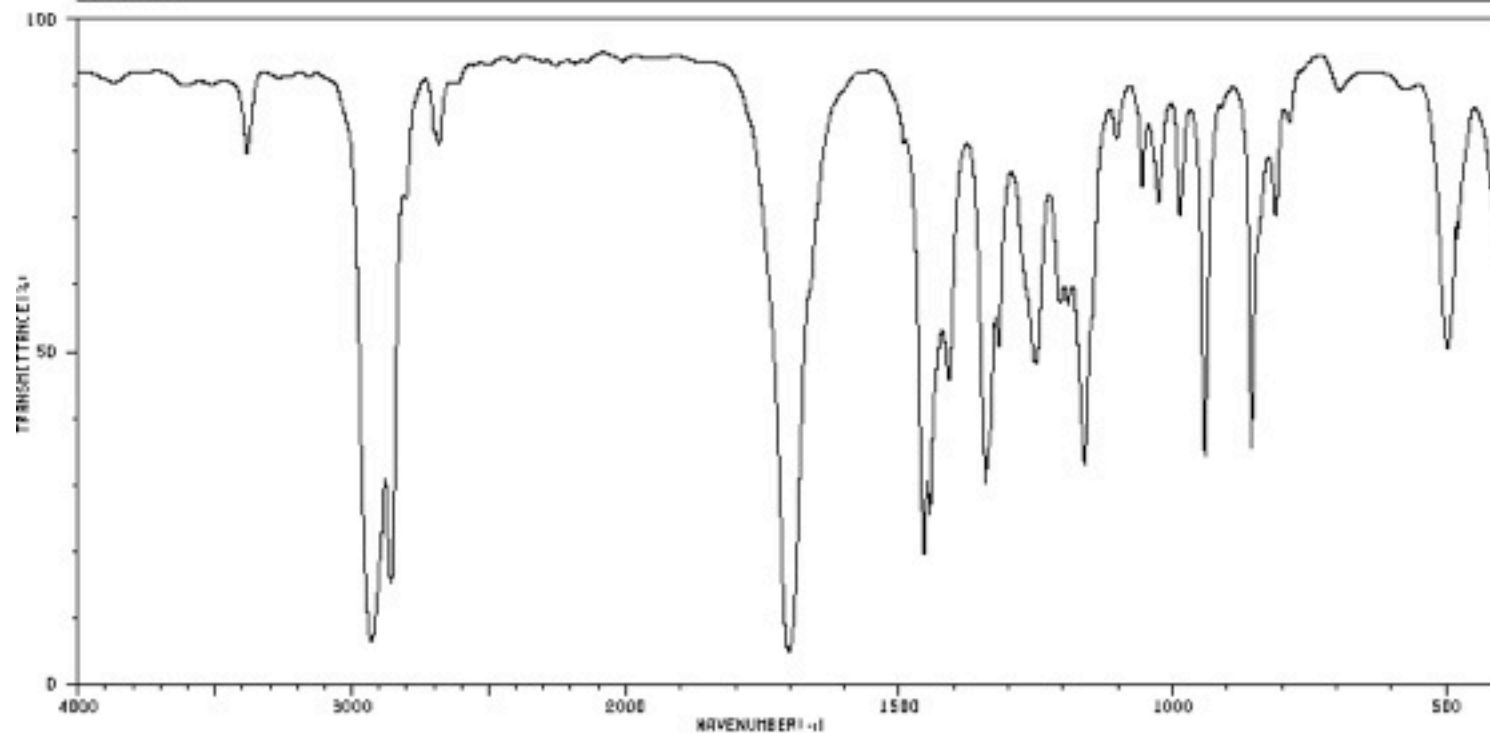
II型

3294	14	1372	20	721	68
3099	35	1299	26	629	53
2946	41	1161	38	599	41
2697	84	1096	72	440	66
1855	4	1042	66		
1563	11	991	82		
1412	21	881	84		

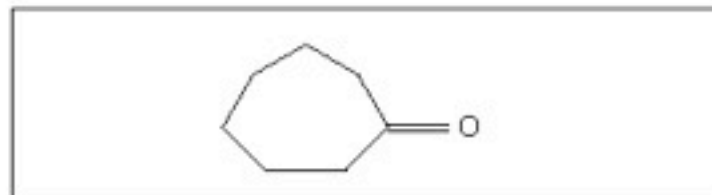


C=O伸縮振動 (7員環ケトン)

HIT-NO=2414 SCORE= () SDBS-NO=3947 IR-NIDA-09927 ; LIQUID FILM
CYCLOHEPTANONE
C₇H₁₂O

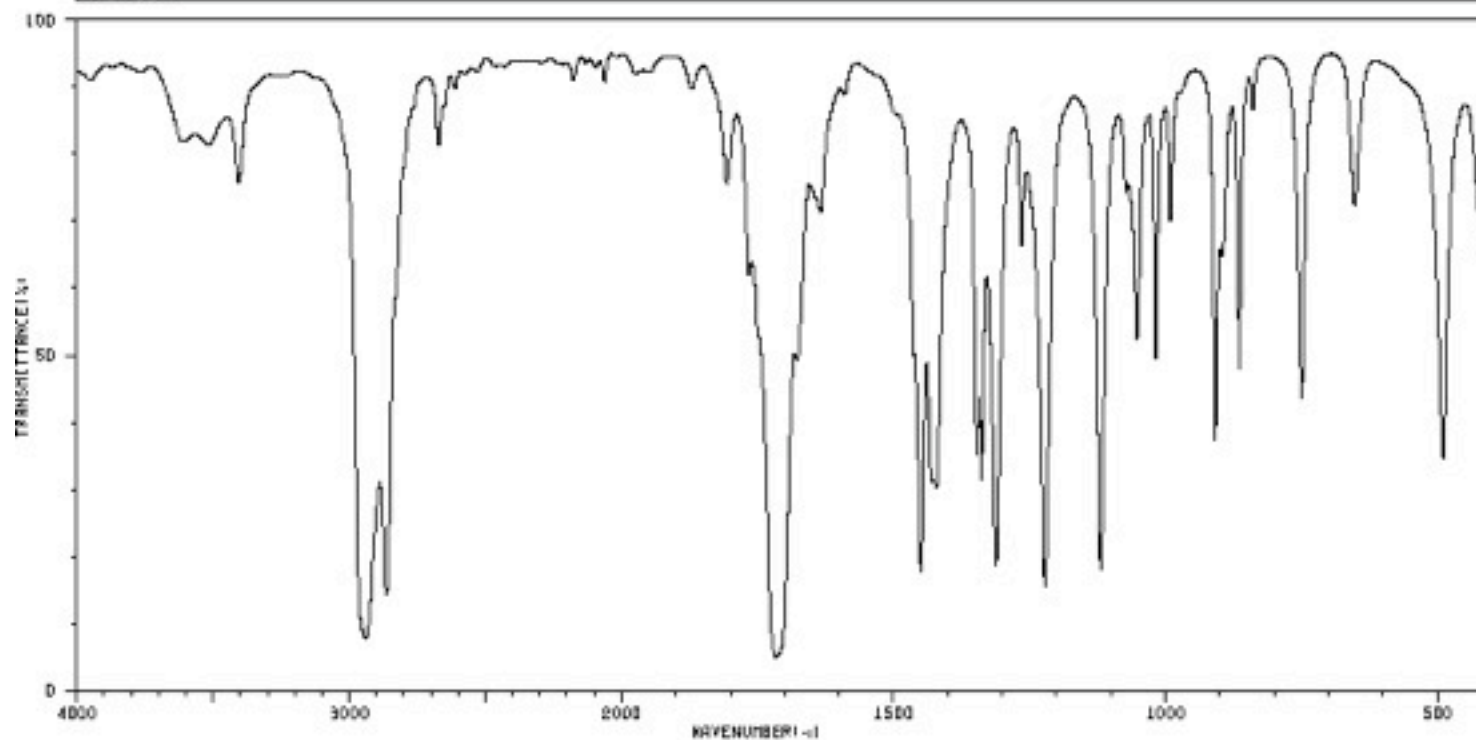


3363	77	1446	24	1161	32	812	68
2928	6	1410	44	1103	79	787	81
2858	14	1343	29	1056	72	696	86
2698	79	1319	49	1026	70	498	49
2681	79	1251	46	987	68	481	64
1702	4	1207	55	941	33		
1455	18	1192	55	856	34		

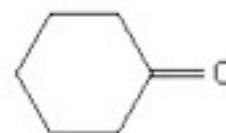


C=O伸縮振動 (6員環ケトン)

HIT-NO=1070 SCORE= () SDBS-NO=571 IR-NIDA-05262 ; LIQUID FILM
CYCLOHEXANONE
C₆H₁₀O

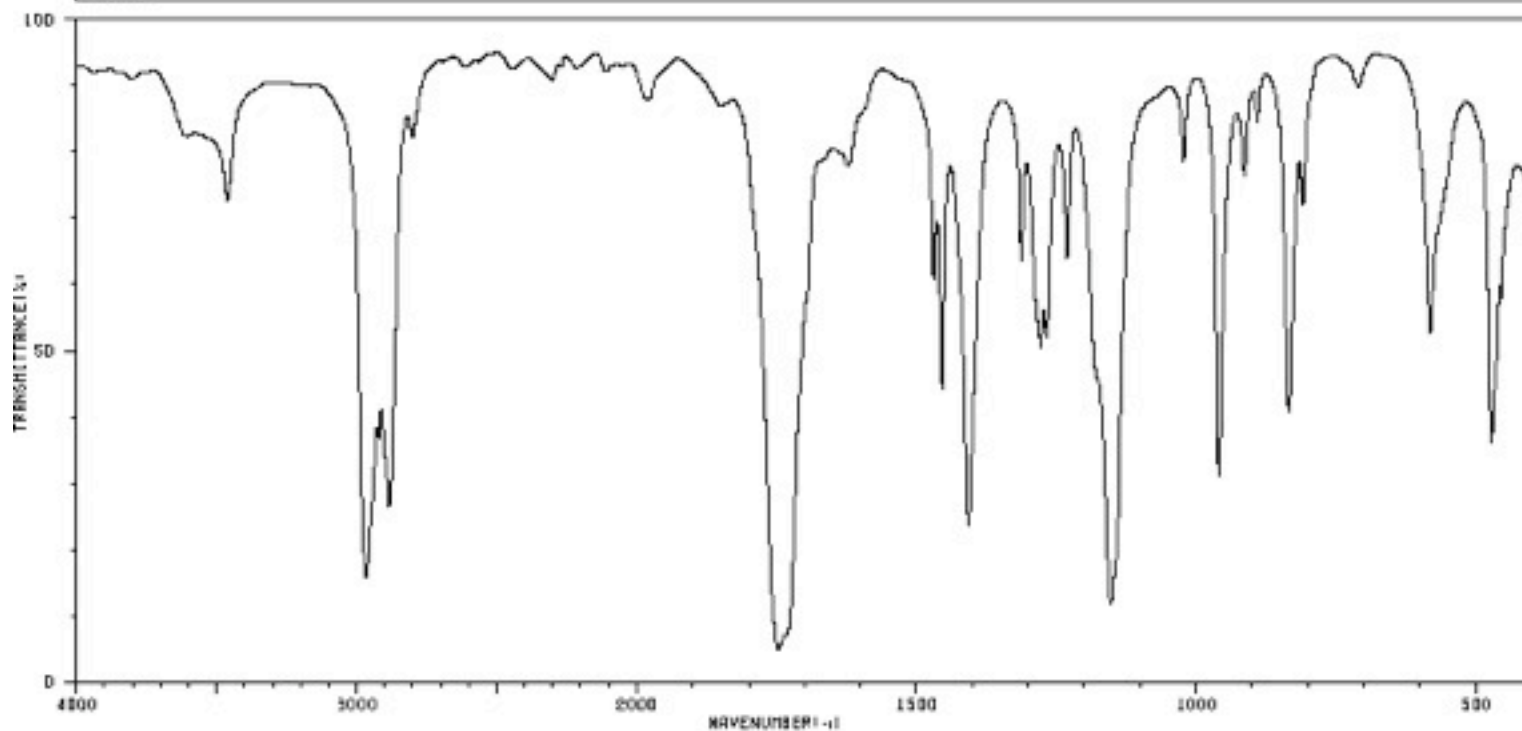


3610	79	2611	86	1460	17	1222	16	896	62
3515	79	1870	86	1429	30	1119	17	864	46
3407	72	1808	72	1422	26	1073	72	839	64
2941	7	1766	60	1347	34	1062	60	760	42
2864	13	1716	4	1338	30	1018	47	652	70
2670	79	1677	47	1311	17	991	68	490	33
2664	84	1634	68	1266	64	909	36		

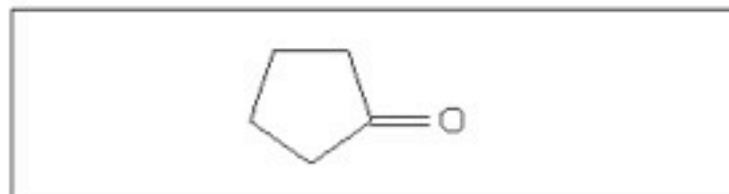


C=O伸縮振動 (5員環ケトン)

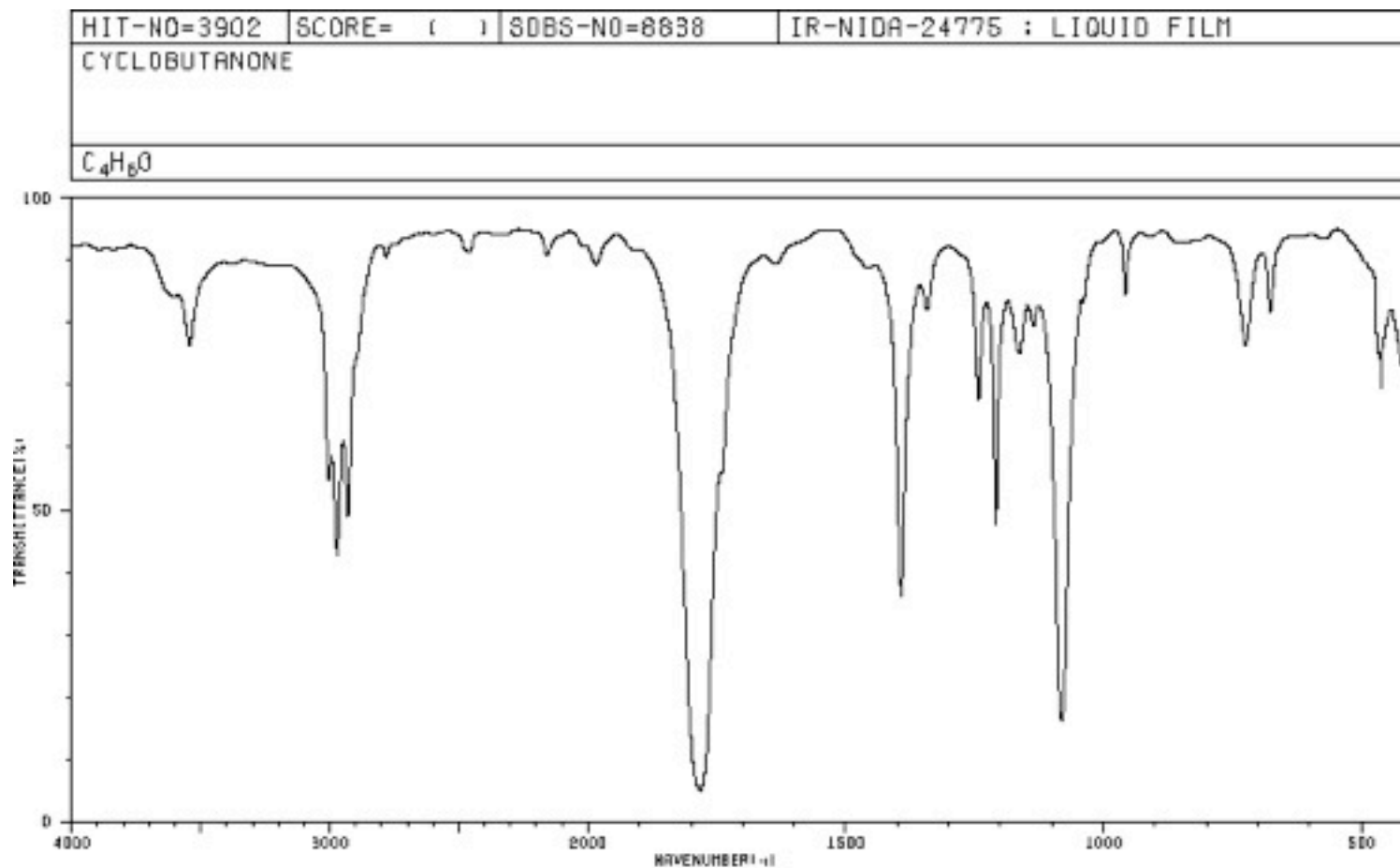
HIT-NO=3870	SCORE= 1	SDBS-NO=7939	IR-NIDA-14413 : LIQUID FILM
CYCLOPENTANONE			
C ₅ H ₈ O			



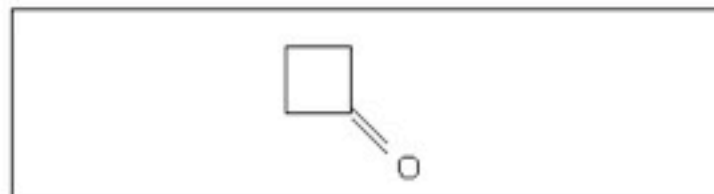
3462	70	1622	74	1231	62	810	70
2966	15	1470	58	1153	11	710	86
2921	35	1455	42	1025	74	582	50
2884	26	1408	22	959	30	473	36
2800	79	1313	60	913	74	463	47
1980	84	1278	48	891	81	457	55
1747	4	1267	50	834	39		



C=O伸縮振動 (4員環ケトン)

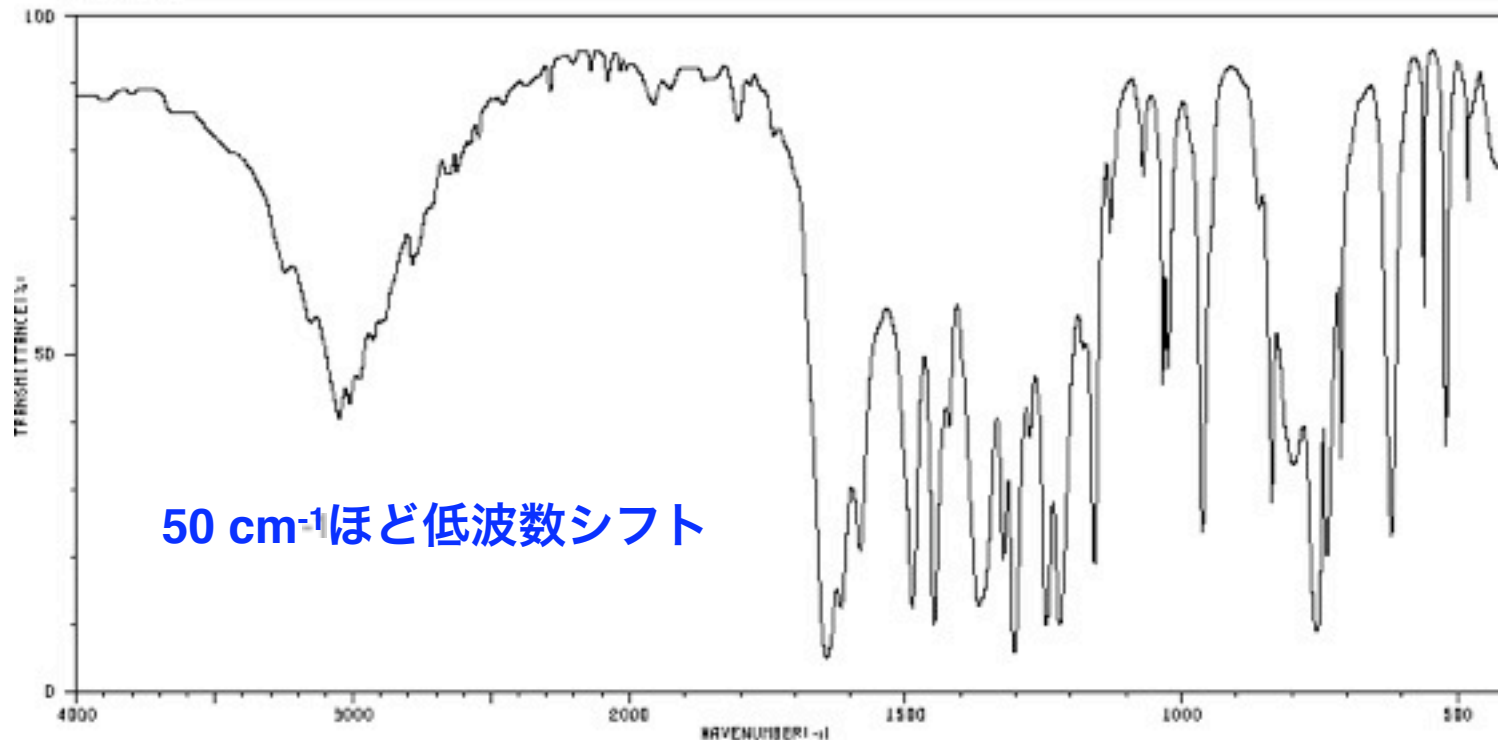


3643	74	1393	34	958	81
3004	52	1343	79	725	72
2971	41	1243	64	877	79
2930	47	1209	48	463	66
1984	86	1164	72		
1783	4	1137	77		
1636	86	1081	15		

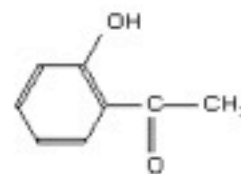


C=O伸縮振動 (水素結合したケトン)

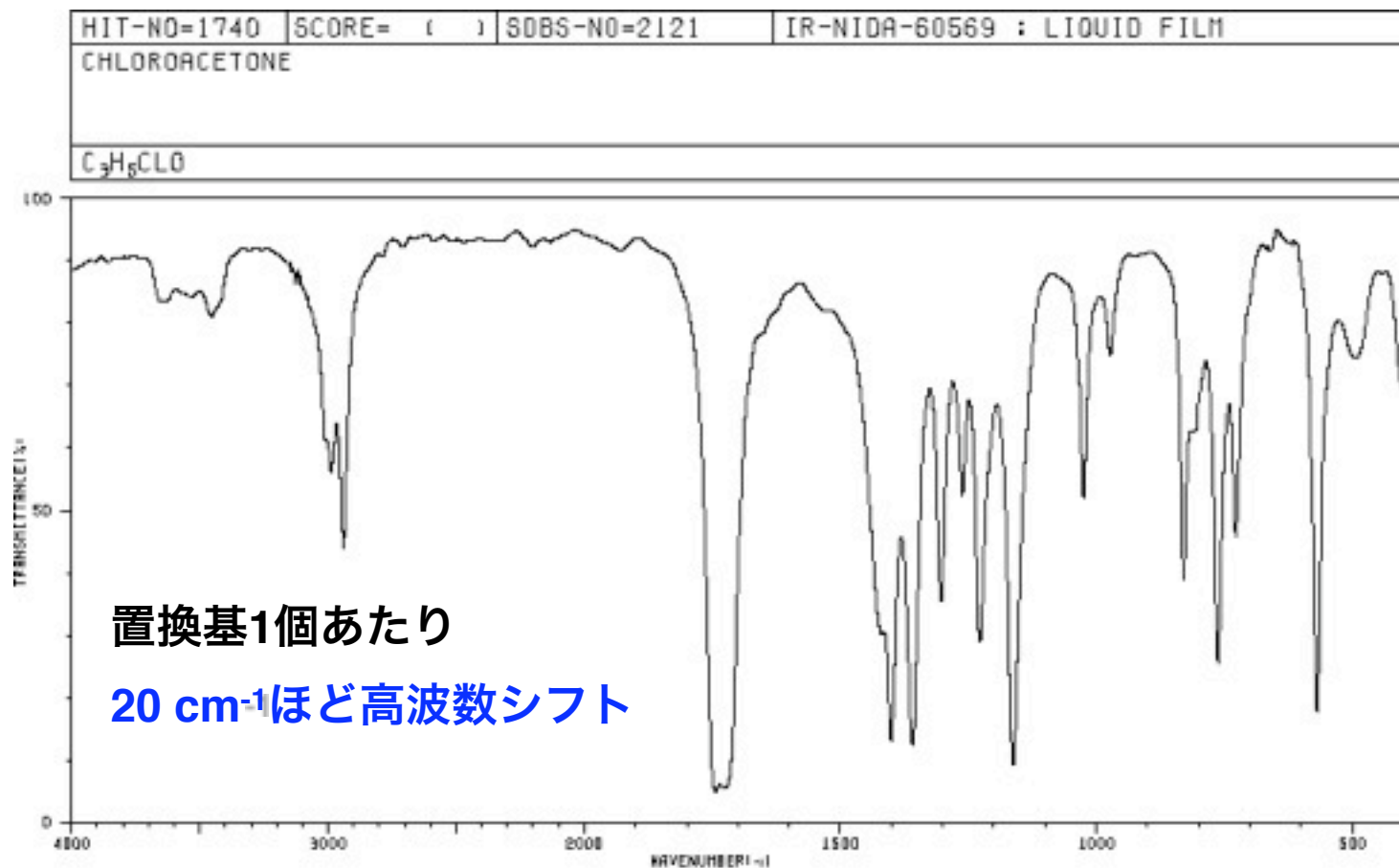
HIT-NO=1154	SCORE= ()	SDBS-NO=724	IR-NIDA-20623 : LIQUID FILM
2'-HYDROXYACETOPHENONE			
C ₈ H ₈ O ₂			



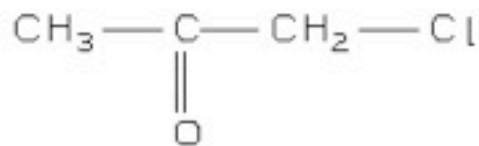
3061	38	1617	12	1303	6	1069	74	765	8
3011	41	1582	20	1275	36	1034	43	737	19
2706	80	1488	12	1245	9	1023	46	712	33
2773	62	1448	9	1221	9	963	22	621	22
2650	74	1421	37	1173	49	860	68	562	55
2623	74	1368	12	1158	18	837	26	522	35
1643	4	1323	18	1129	66	797	32	492	70



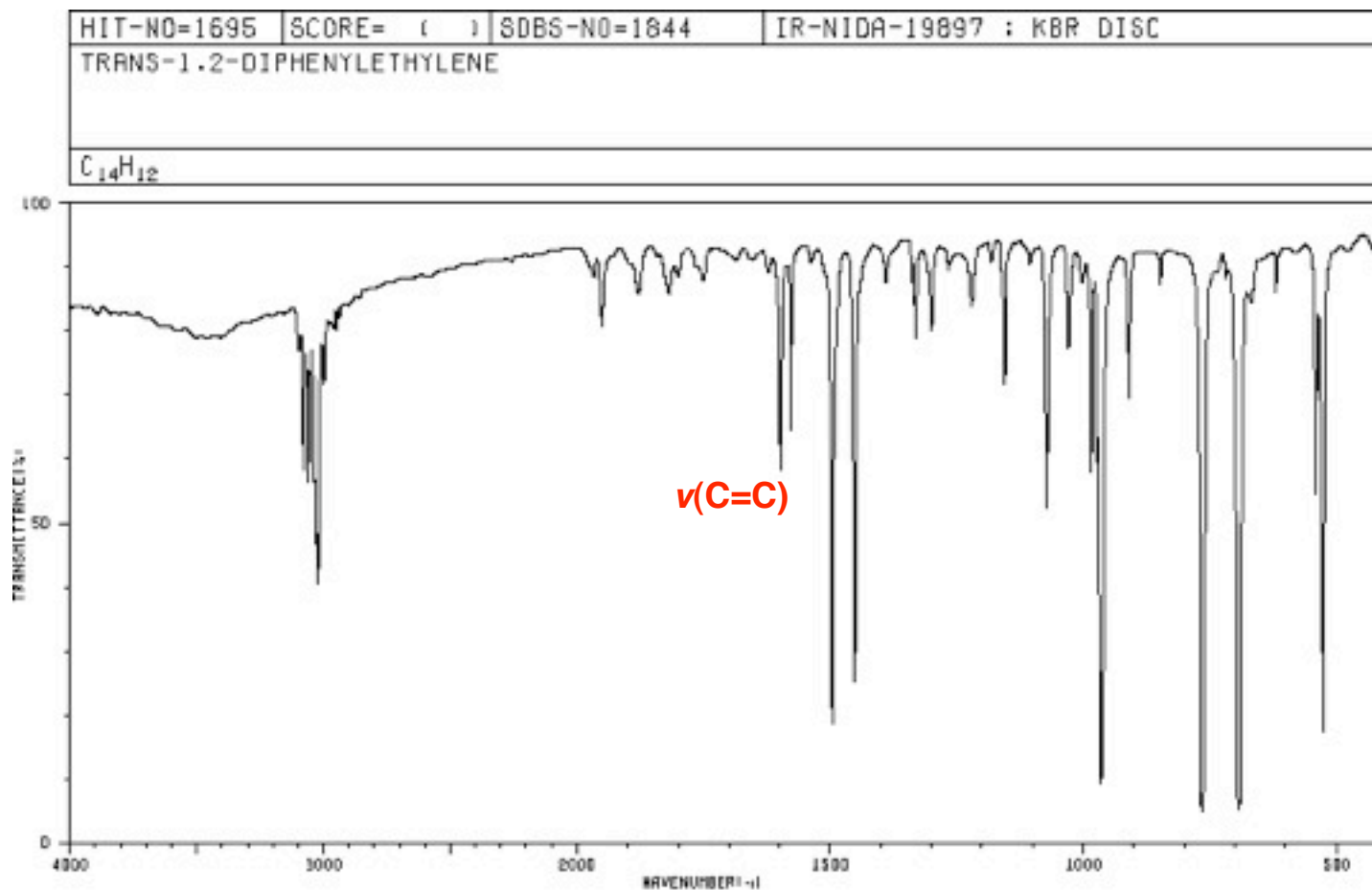
C=O伸縮振動 (α 位に電子吸引基)



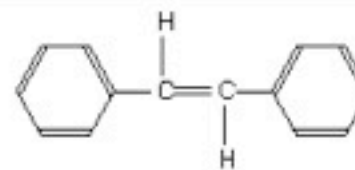
3660	79	2996	67	1416	29	1163	9	728	44
3640	81	2985	53	1401	12	1036	72	569	17
3629	81	2973	60	1360	12	1025	50	494	72
3466	79	2938	42	1304	34	973	72		
3127	84	1744	4	1267	57	831	37		
3117	84	1734	5	1262	50	612	60		
3007	68	1726	6	1229	27	763	24		



C=C (alkenes) 伸縮振動 (1650 cm⁻¹ ~ 1500 cm⁻¹)

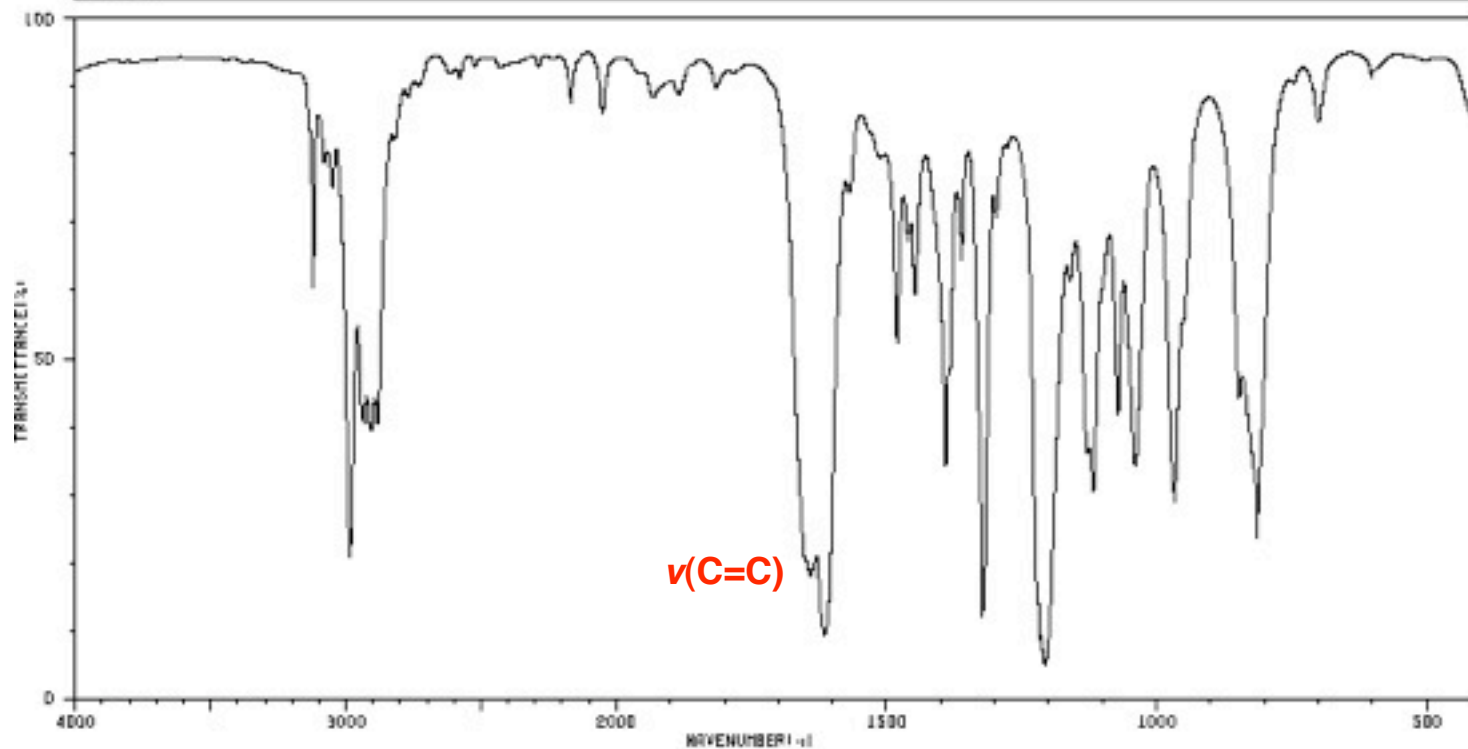


3892	79	2968	77	1678	62	1152	84	910	66
3095	74	2947	77	1496	17	1155	68	848	84
3079	55	2938	78	1452	23	1073	50	767	4
3060	63	1960	77	1390	84	1030	74	693	4
3034	52	1878	81	1332	77	985	55	669	81
3021	38	1817	81	1300	77	973	57	541	52
2998	68	1698	65	1221	81	966	8	626	16



C=C伸縮振動 (enol ether)

HIT-NO=1758	SCORE= ()	SOBS-NO=2152	IR-NIDA-02887 ; LIQUID FILM
ETHYL VINYL ETHER			
C ₄ H ₈ O			

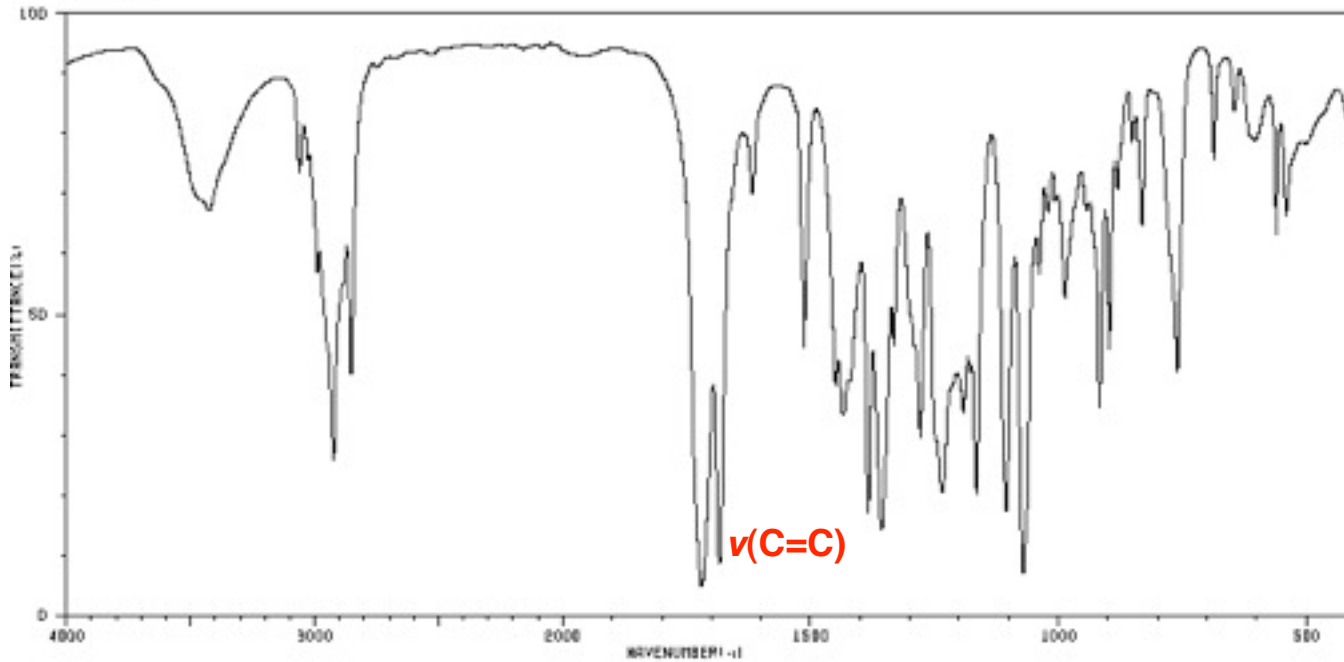


3136	79	2883	38	1614	9	1352	62	1117	29
3121	58	2168	84	1568	72	1322	12	1072	39
3080	77	2052	81	1481	50	1298	68	1039	33
3049	72	1932	84	1461	64	1216	8	966	27
2984	20	1884	86	1447	57	1207	4	848	42
2934	36	1818	86	1391	33	1150	58	814	22
2907	37	1641	17	1383	46	1128	36	700	81

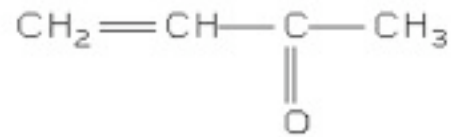
CH3-CH2-O-CH=CH2

C=C伸縮振動 (conjugated alkenes)

HIT-NO=2461	SCORE= ()	SDBS-NO=4018	IR-NIDA-03609 : LIQUID FILM
3-BUTEN-2-ONE			
C ₄ H ₆ O			

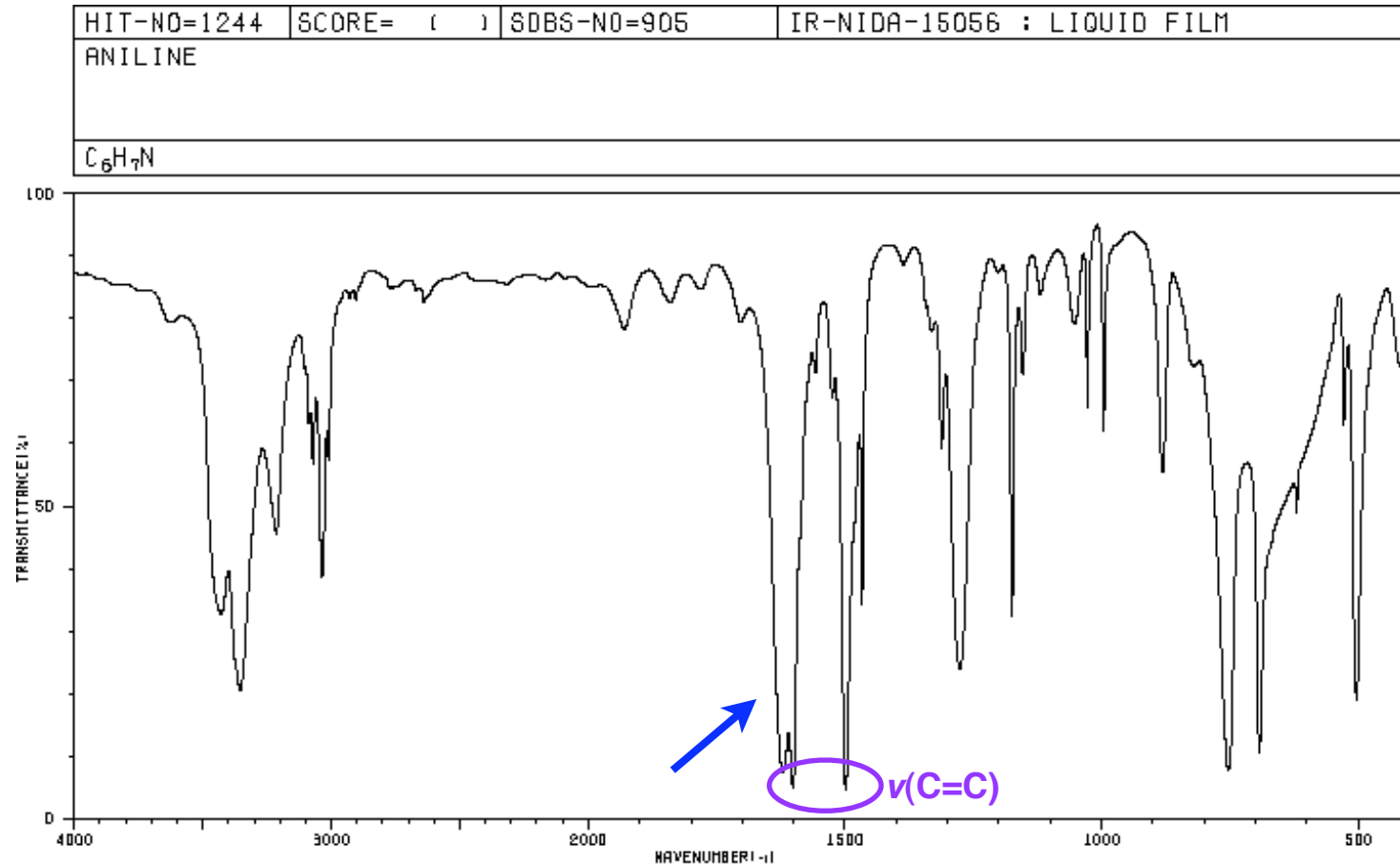


3426	64	1616	68	1333	43	1039	66	662	77
3061	70	1513	42	1279	28	1021	64	632	62
2900	55	1450	37	1235	19	987	50	760	38
2924	24	1434	32	1192	32	942	64	687	72
2852	38	1423	37	1166	19	917	33	604	77
1720	4	1384	15	1105	16	898	42	561	60
1683	8	1367	13	1071	6	881	68	541	64

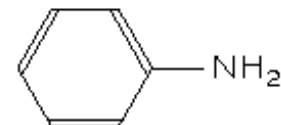


N-H変角振動 (1650~1500 cm⁻¹)

(第二級アミンは弱い、アンモニウム塩は強い)



3623	77	3010	67	1706	77	1332	74	996	60
3429	32	2930	81	1621	7	1312	57	881	53
3354	20	2904	79	1601	5	1277	29	754	8
3214	44	2640	79	1557	70	1176	32	693	10
3088	62	2627	81	1525	66	1154	68	620	47
3072	55	1929	77	1498	4	1053	77	529	60
3037	38	1839	79	1467	34	1028	64	504	18



$1500\text{ cm}^{-1} \sim 600\text{ cm}^{-1}$

(指紋領域: 複雑)

ν (**NO**): $1550 \sim 1350\text{ cm}^{-1}$ (**nitro, nitroso groups**)

ν (**SO**): $1350 \sim 1120\text{ cm}^{-1}$ (**sulfones, sulfoxides**)

ν (**C-O**): $1300 \sim 1000\text{ cm}^{-1}$ (**alcohols, ethers, esters**)

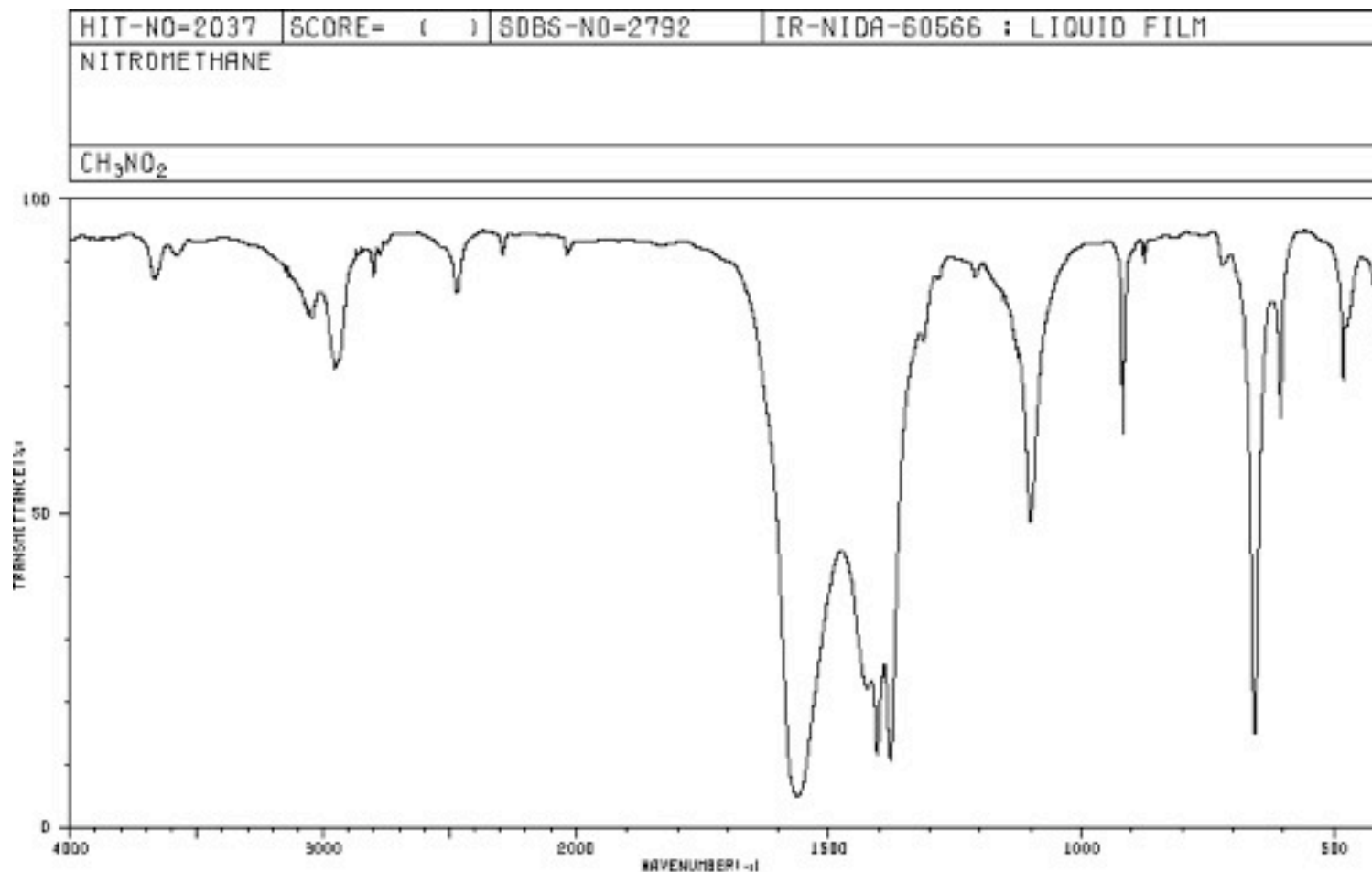
δ (**CH**): $1000 \sim 680\text{ cm}^{-1}$ (**alkenes, aromatics**)

★ ケトンとエステルの区別

★ ベンゼンの置換パターン

★ アルケンの置換パターン

NO伸縮振動 (NO₂, 2本)

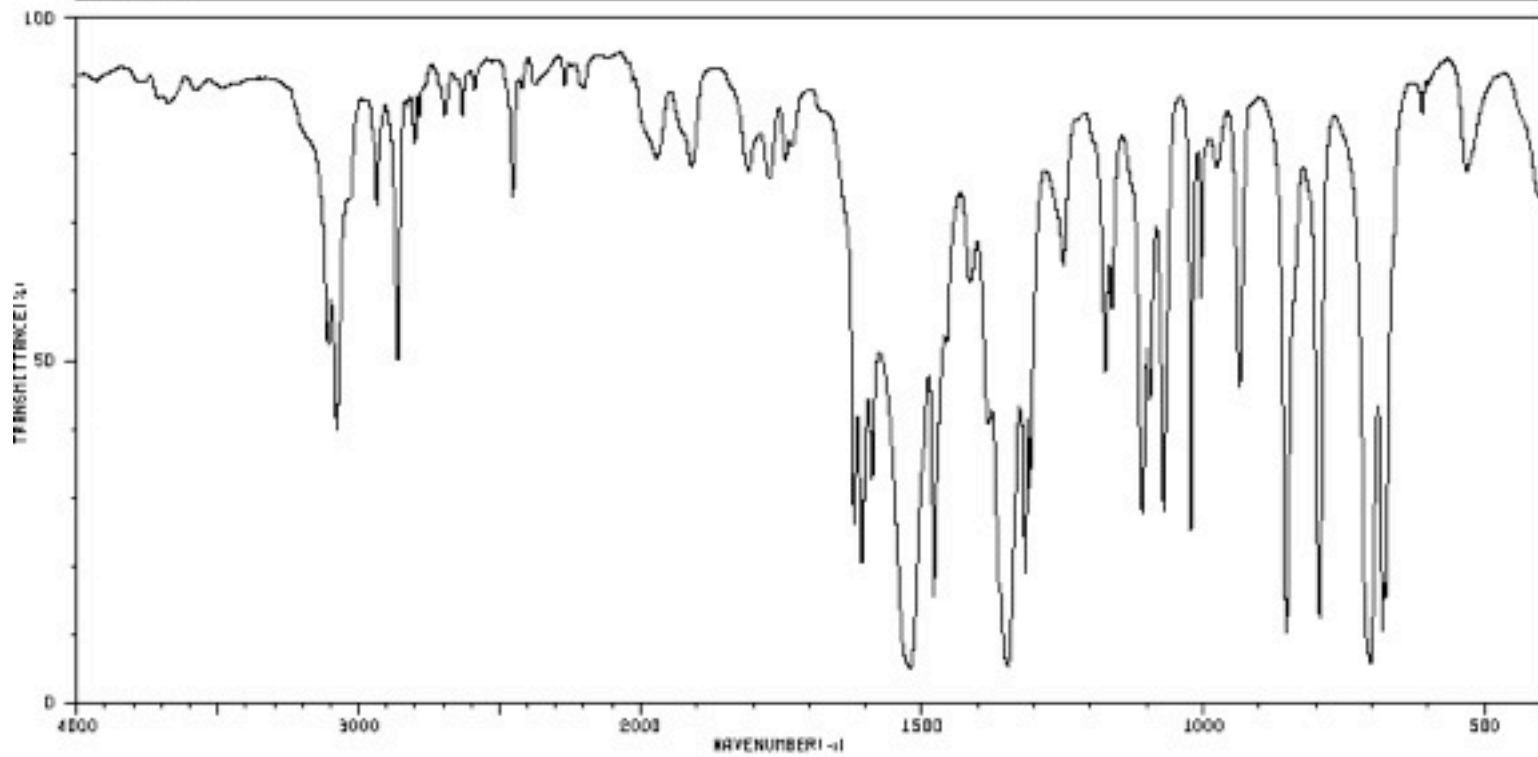


3666	84	2802	84	1211	84	606	62
3140	84	2469	81	1157	81	482	68
3064	79	1562	4	1101	46		
3061	79	1423	21	916	60		
3041	77	1404	10	876	86		
2956	70	1378	10	720	86		
2932	72	1312	74	667	14		

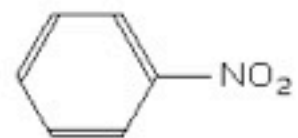
CH₃NO₂

NO伸縮振動 (NO₂, 2本)

HIT-NO-1059 SCORE= () SDBS-NO-552 IR-NIDA-05130 : LIQUID FILM
 NITROBENZENE
 C₆H₅NO₂

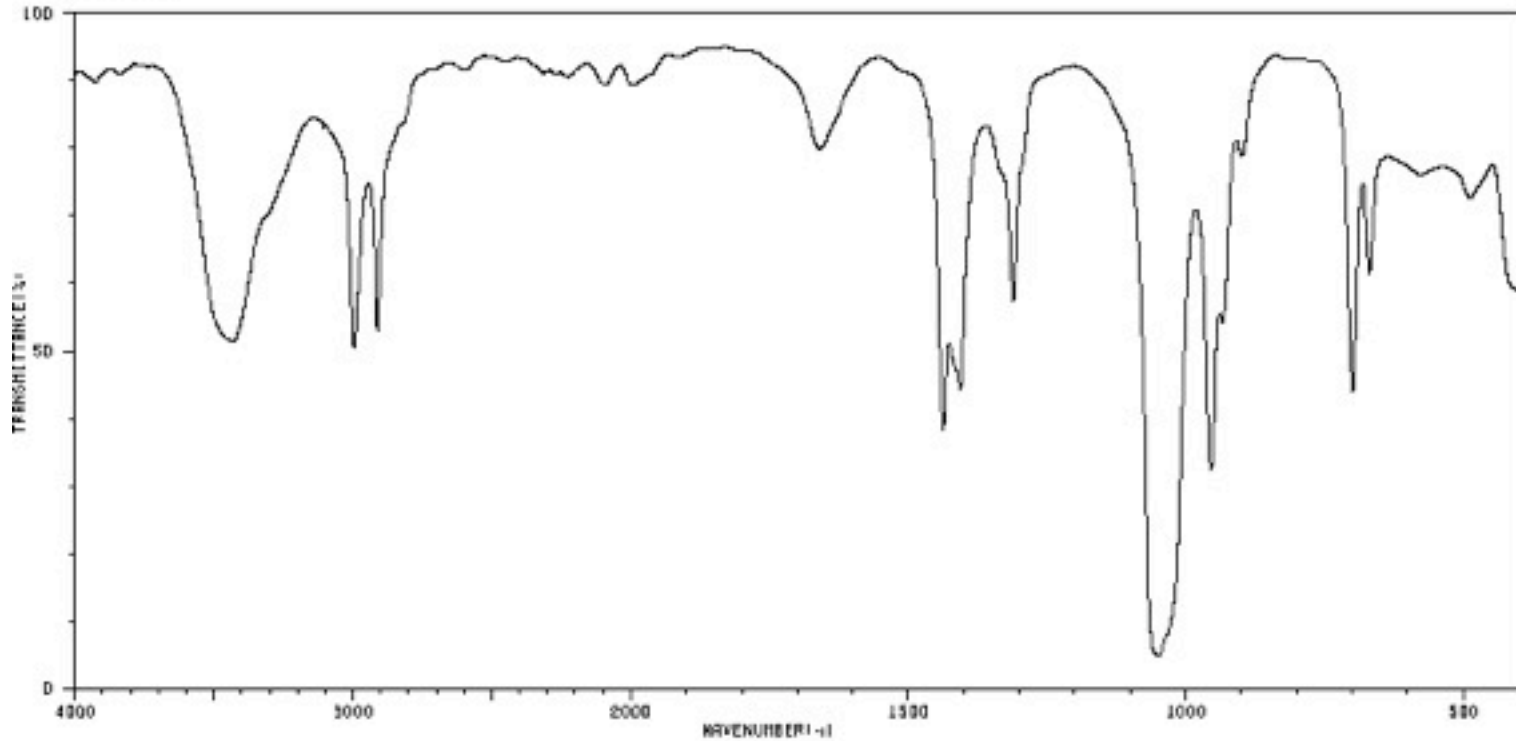


3108	60	1772	74	1416	68	1176	46	976	74
3078	38	1620	25	1382	39	1163	55	935	44
2935	70	1607	20	1363	17	1108	26	852	10
2861	49	1589	31	1347	6	1096	42	794	12
2453	72	1521	4	1317	18	1070	26	703	5
1906	74	1479	14	1305	30	1022	24	682	10
1808	74	1466	60	1248	62	1004	67	676	14

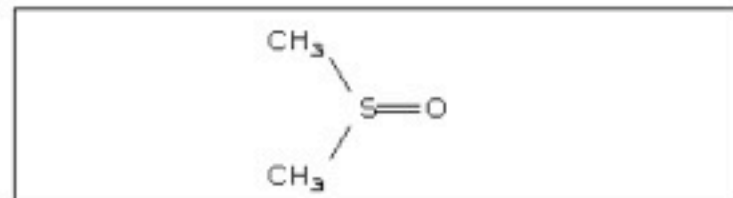


SO伸縮振動 (sulfoxide)

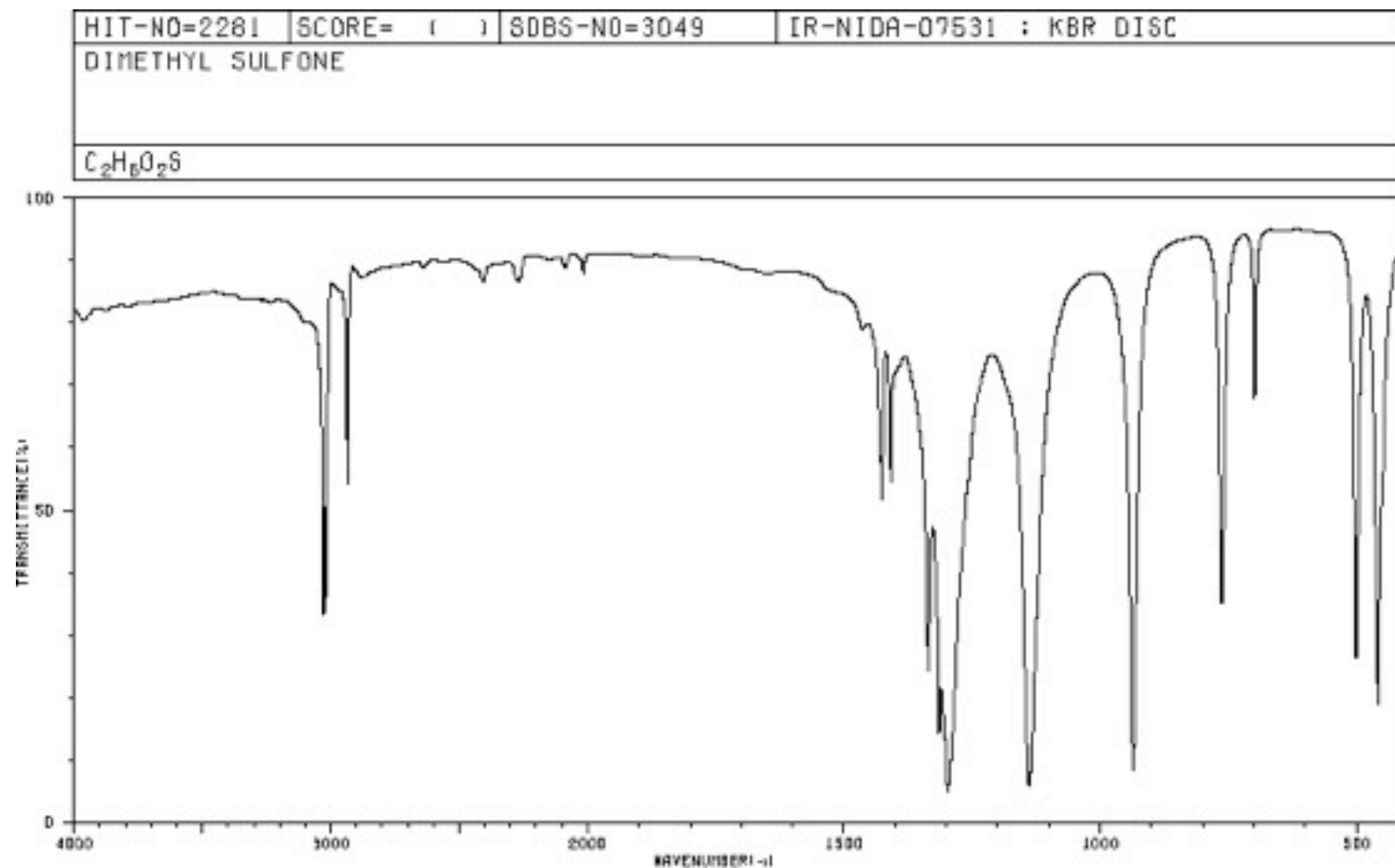
HIT-NO=1916 SCORE= () SDBS-NO=2459 IR-NIDA-63111 : LIQUID FILM
DIMETHYL SULFOXIDE
C2H6OS



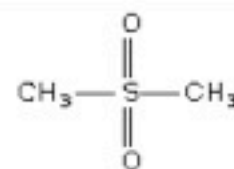
3928	86	1994	86	934	62
3446	50	1659	77	898	77
3434	49	1437	37	700	42
2996	49	1407	49	670	68
2913	50	1311	55	488	70
2091	86	1050	4		
1999	86	966	31		



SO伸縮振動 (sulfones, 2本)

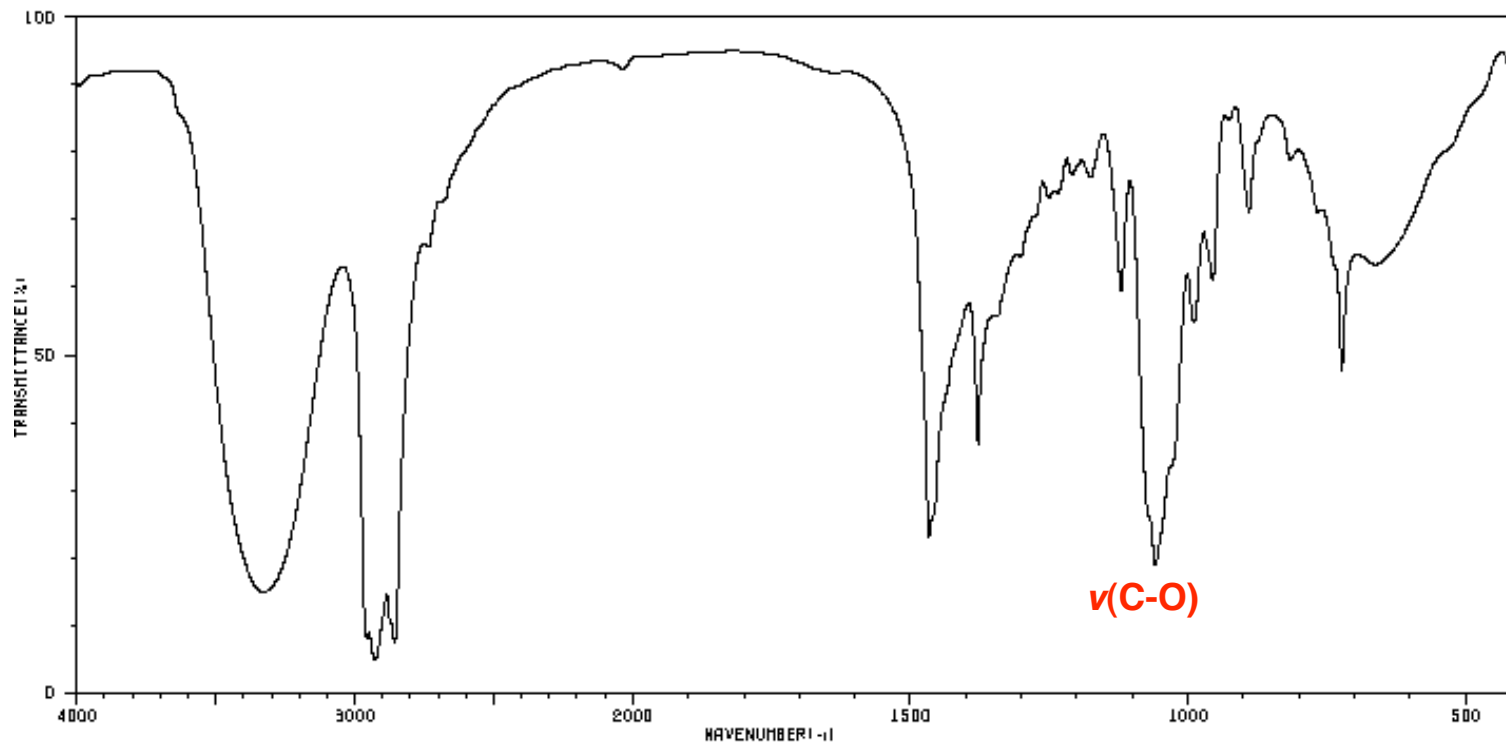


3026	32	2086	86	1298	4
3017	35	2016	84	1139	5
2934	52	1428	50	936	8
2879	84	1409	52	764	34
2641	84	1401	68	699	66
2404	84	1338	29	502	25
2269	84	1316	19	469	18



C-O伸縮振動 (alcohol)

HIT-NO=1673	SCORE= ()	SDBS-NO=1938	IR-NIDA-07946 : LIQUID FILM
1-OCTANOL			
<chem>C8H18O</chem>			

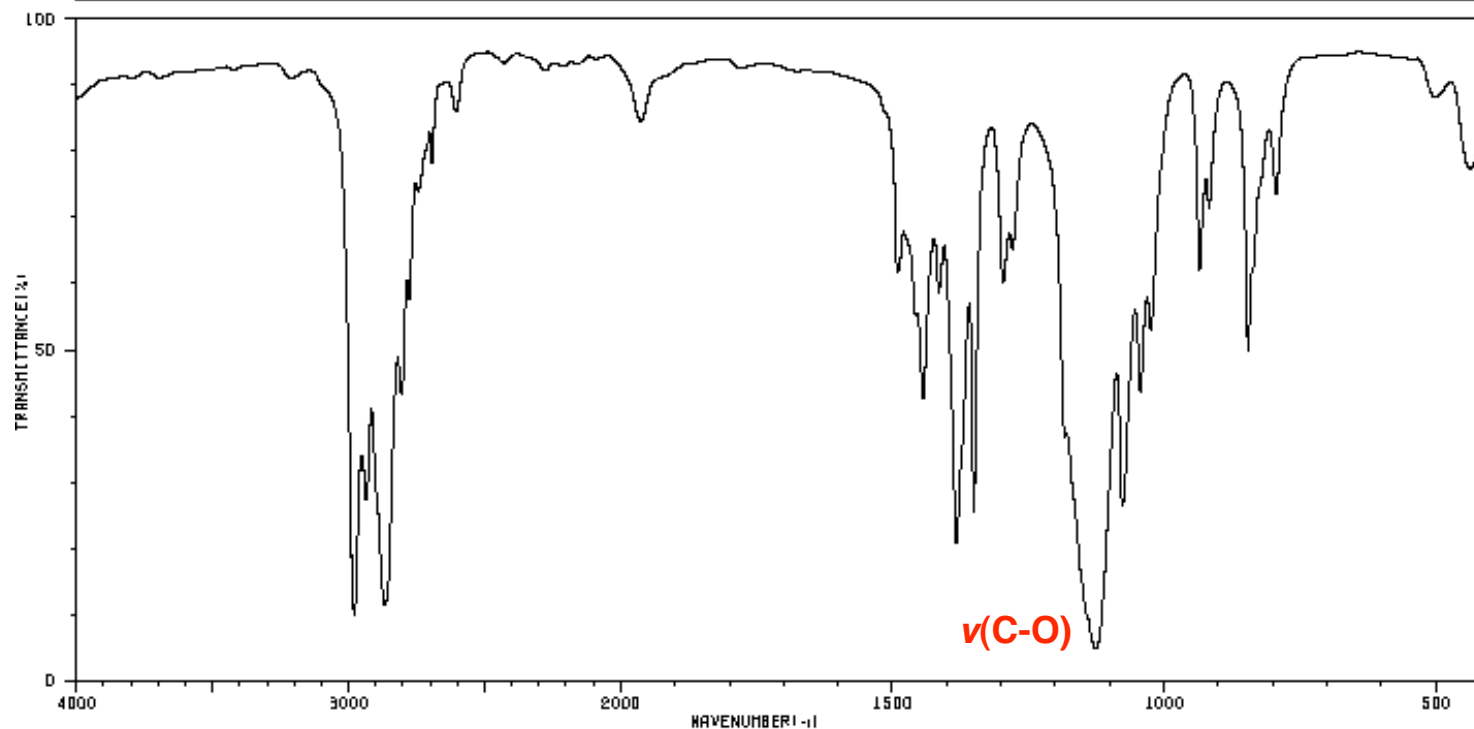


3338	14	1246	70	956	58
3327	14	1235	70	890	68
2927	4	1209	74	818	77
2870	10	1176	74	723	46
2856	7	1120	57	662	60
1467	21	1059	18		
1379	35	989	62		

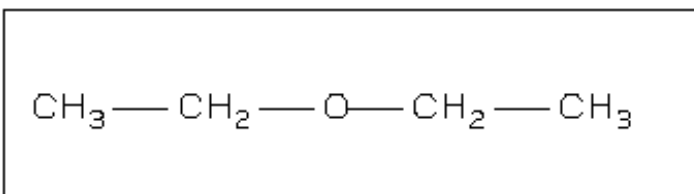


C-O伸縮振動 (ether)

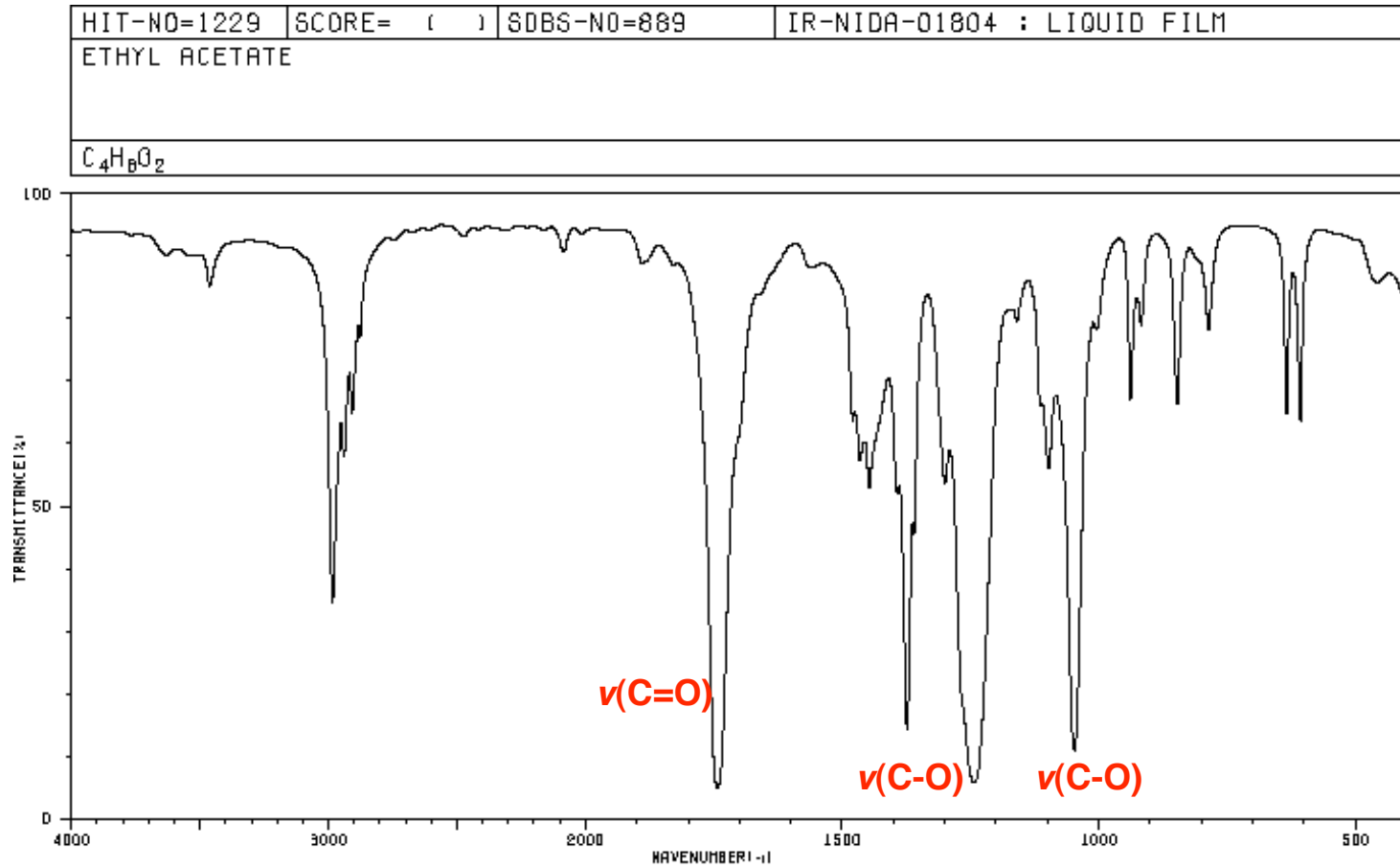
HIT-NO=1756	SCORE= ()	SDBS-NO=2150	IR-NIDA-03139 : LIQUID FILM
DIETHYL ETHER			
C ₄ H ₁₀ O			



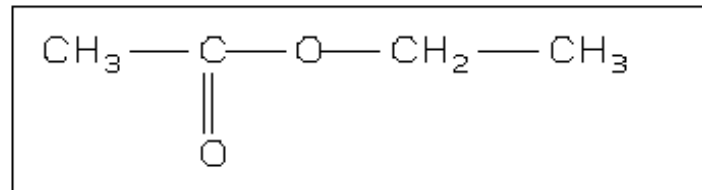
2989	17	2693	74	1389	20	1024	60
2979	9	2604	81	1351	24	935	58
2935	26	1962	81	1297	58	917	68
2868	10	1490	68	1279	62	846	47
2804	41	1457	53	1126	4	794	70
2777	55	1444	41	1077	25	501	84
2743	70	1416	67	1043	42	498	74



C-O伸縮振動 (ester, 2本)

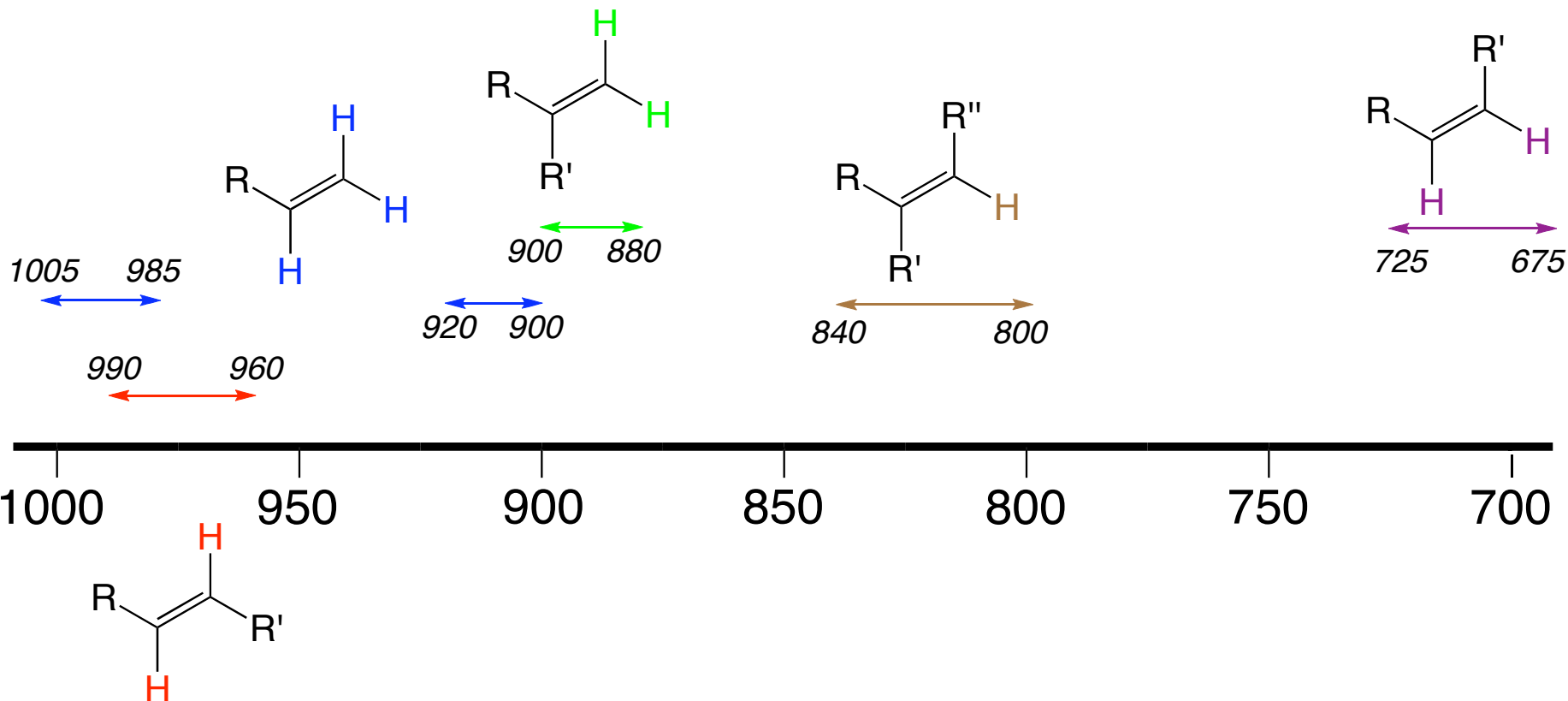


3462	81	1480	60	1243	6	847	64
2983	33	1466	55	1160	77	786	74
2940	55	1448	50	1111	84	634	62
2908	62	1393	60	1098	63	608	60
2877	74	1374	13	1048	10	457	81
1889	86	1360	49	939	84		
1743	4	1301	62	917	77		



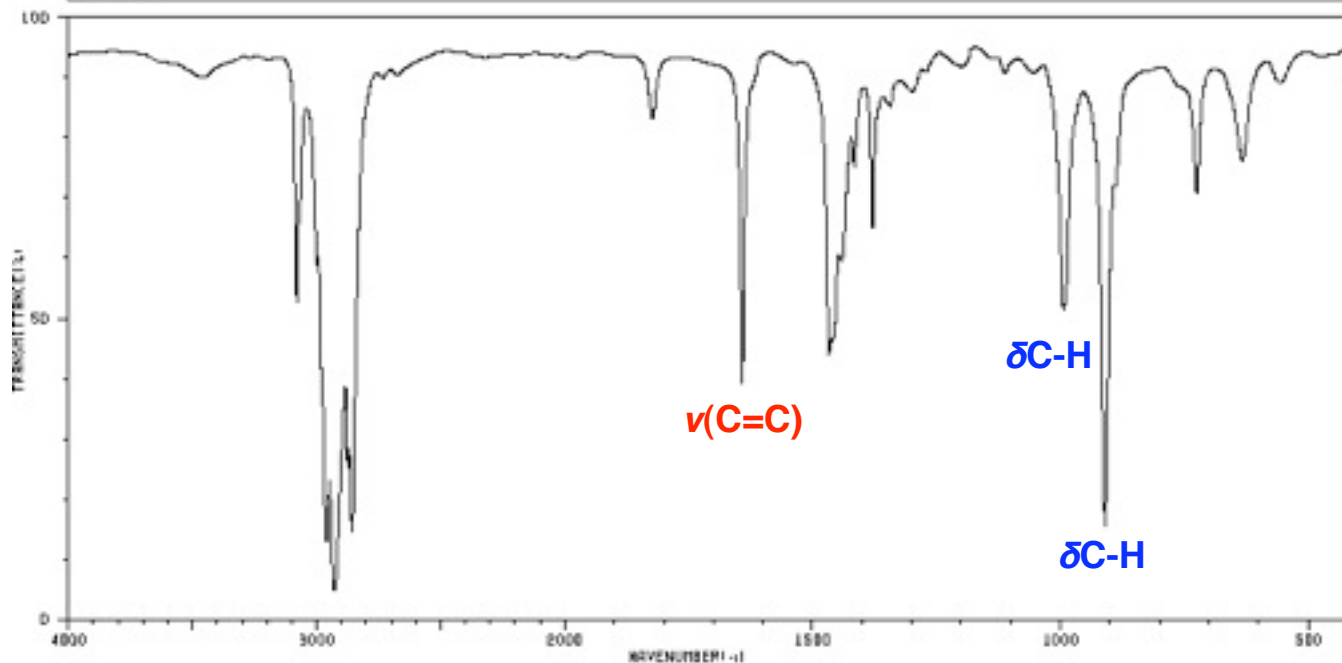
置換パターンに関する情報 (1)

(C=C)

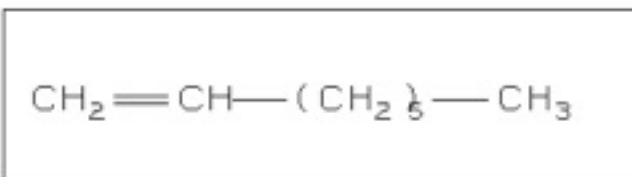


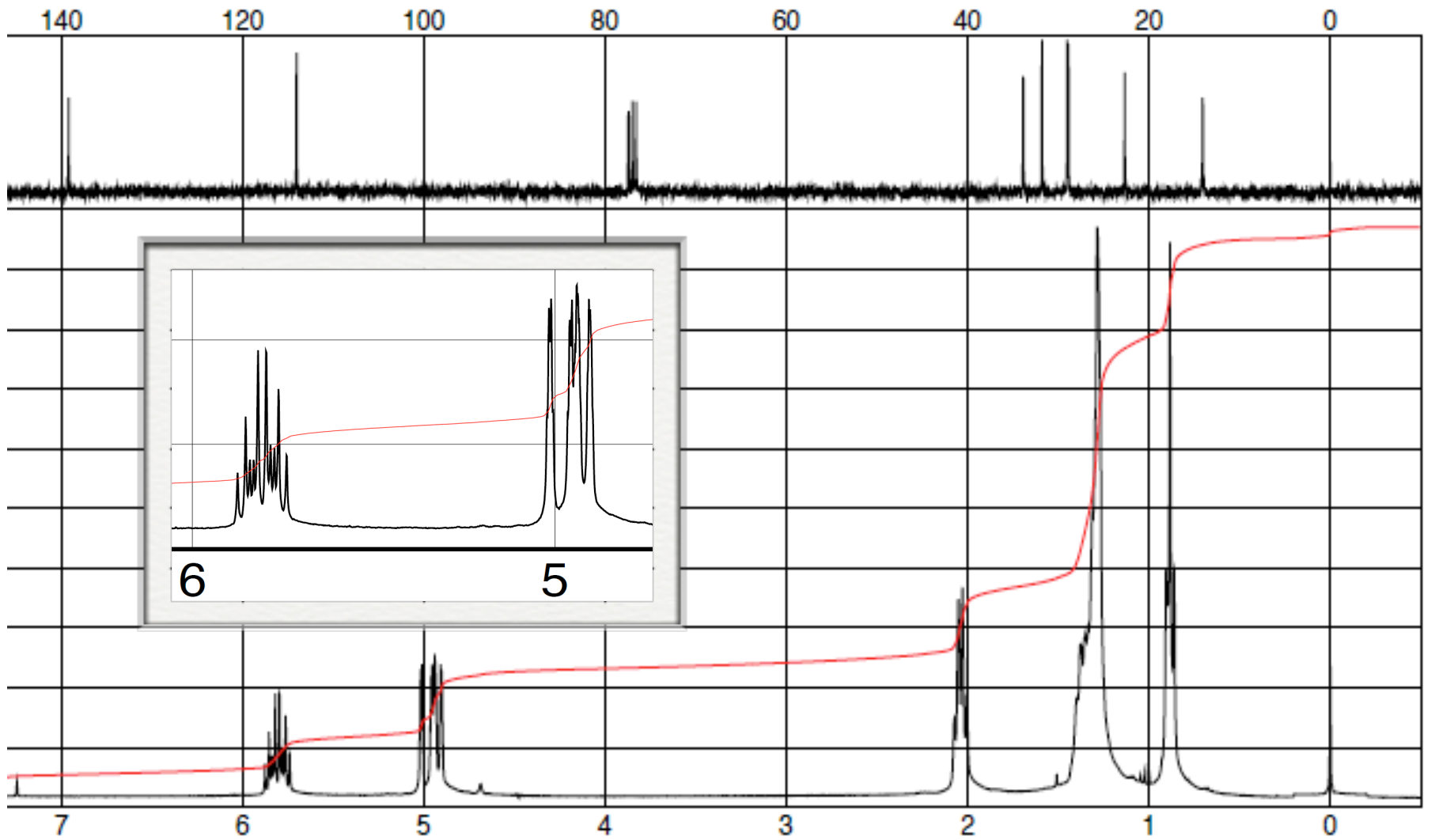
C-H変角振動 (terminal alkenes)

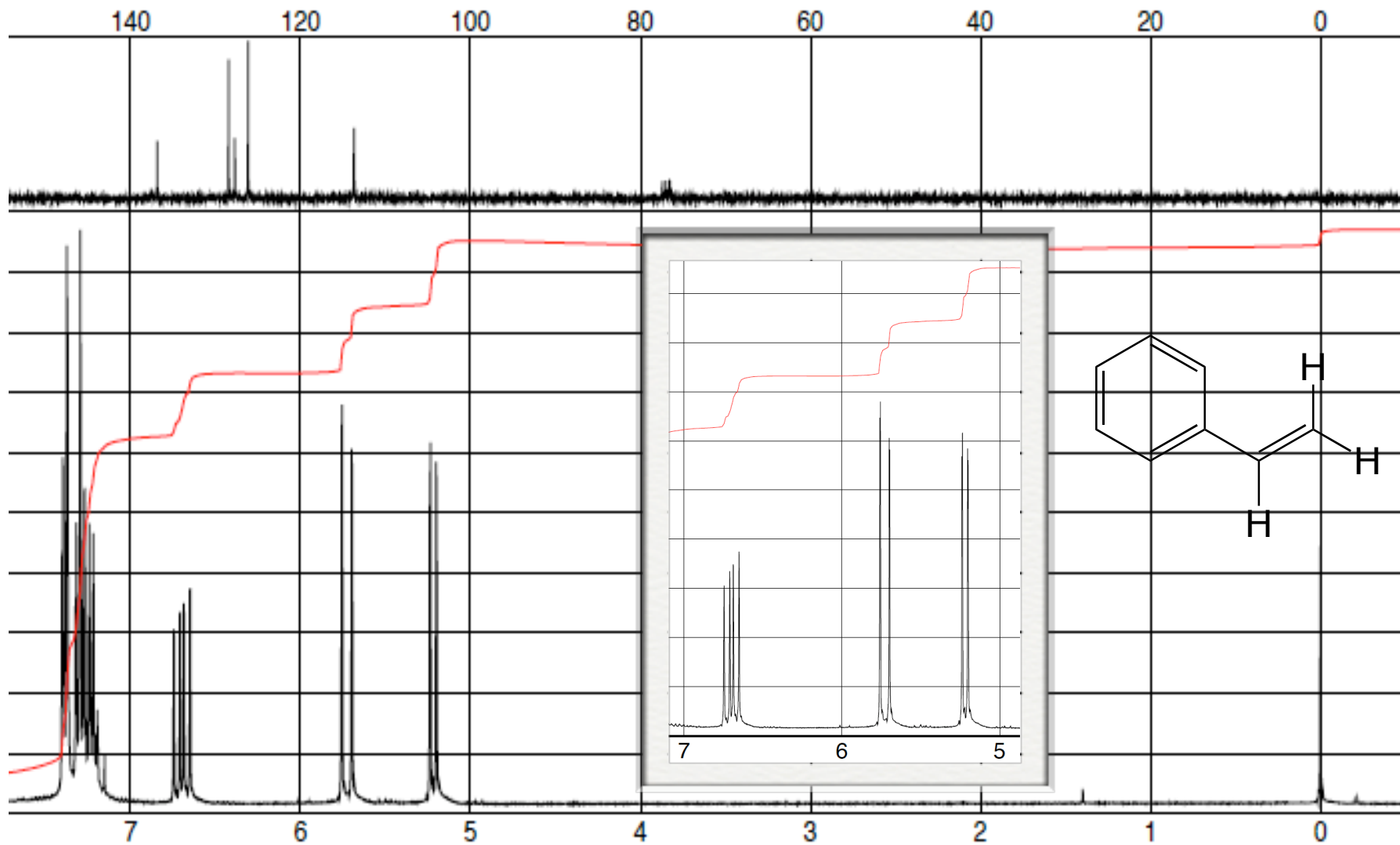
HIT-NO=1179	SCORE= ()	SDBS-NO=788	IR-NIDA-04793 : LIQUID FILM
1-OCTENE			
C_8H_{16}			



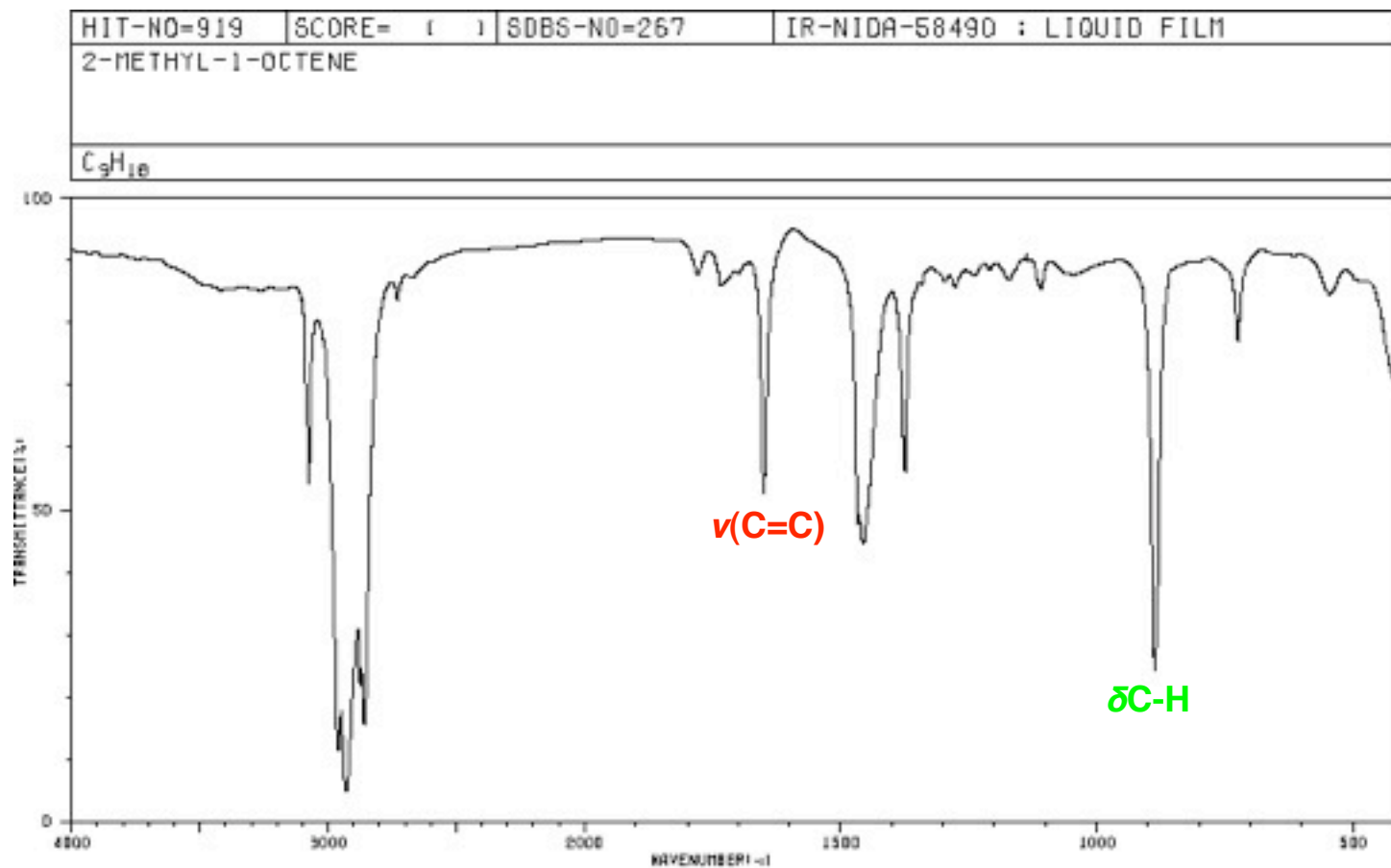
3079	60	1642	37	994	49
2998	57	1468	42	910	14
2959	12	1450	44	725	88
2928	4	1416	72	639	72
2874	23	1379	62	558	86
2857	13	1344	81		
1823	79	1299	84		



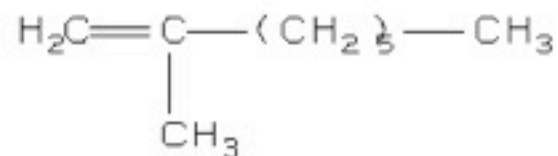


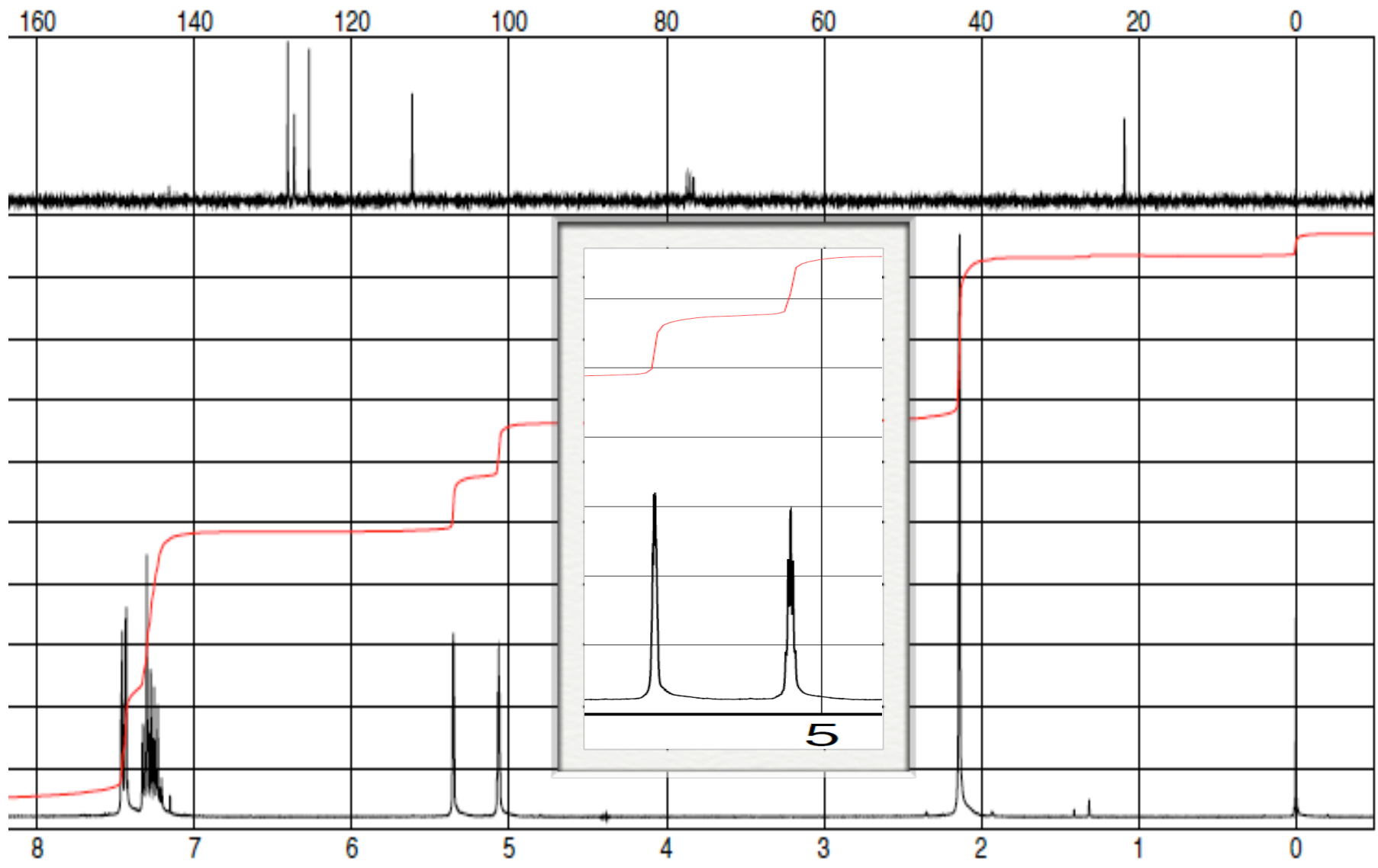


C-H変角振動 (2,2-disubstituted alkenes)

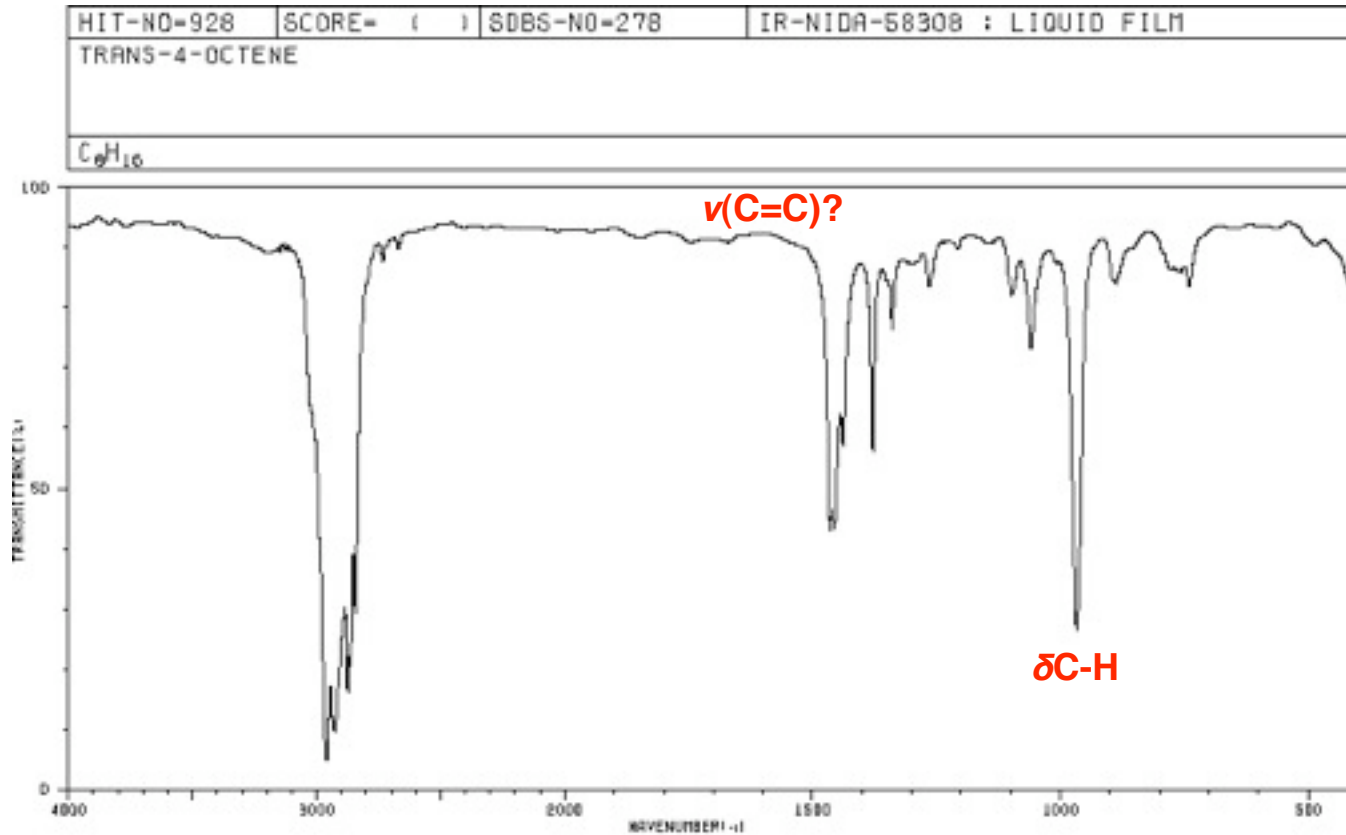


3076	62	1734	84	1173	84
2959	11	1725	84	1109	81
2930	4	1651	50	867	25
2874	21	1467	46	726	74
2859	15	1456	43	545	81
2729	81	1378	53		
1780	84	1278	81		

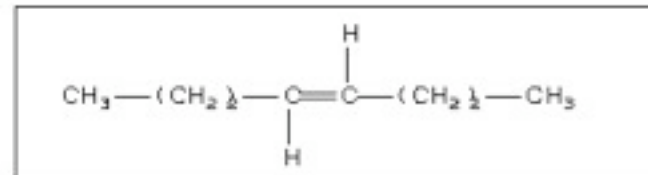


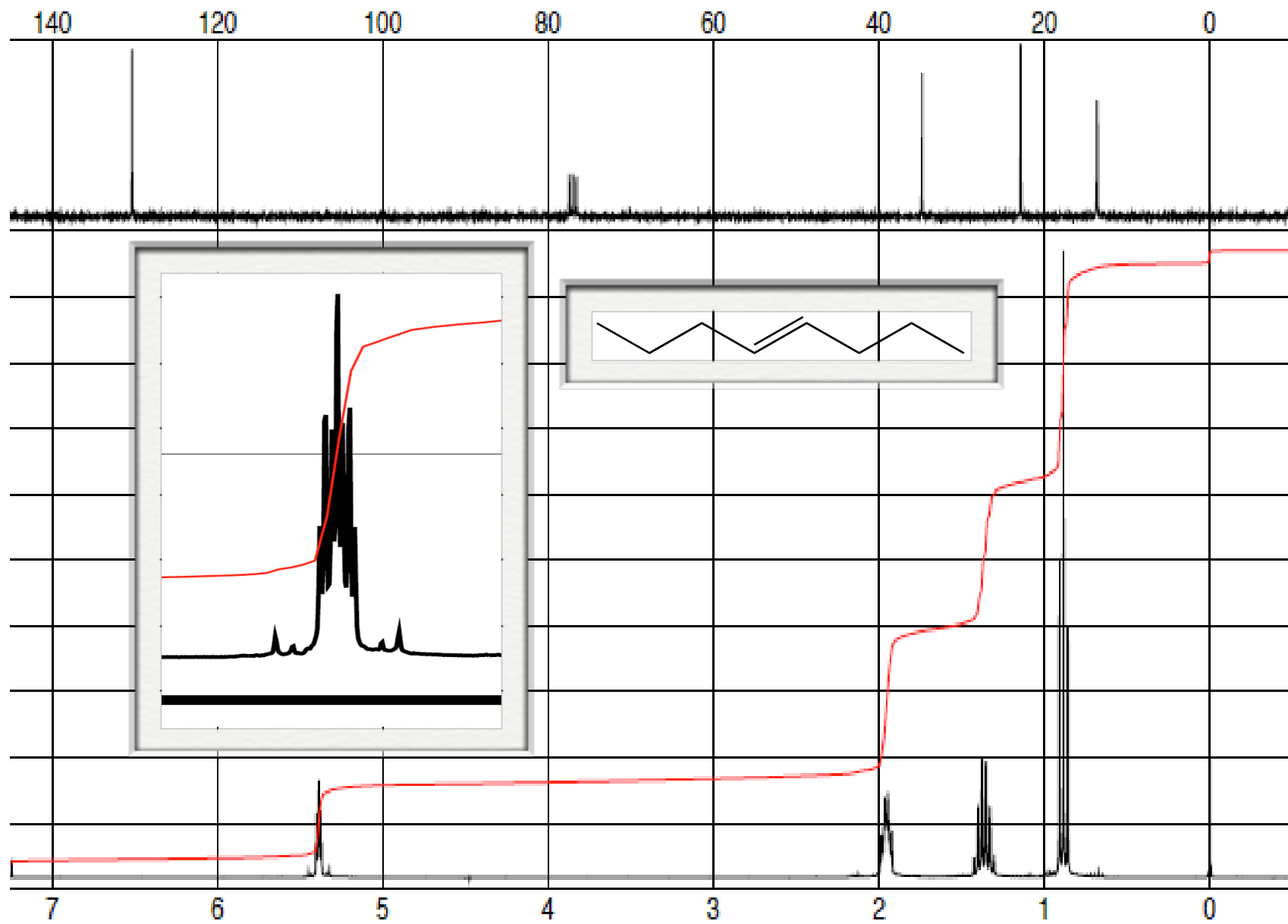


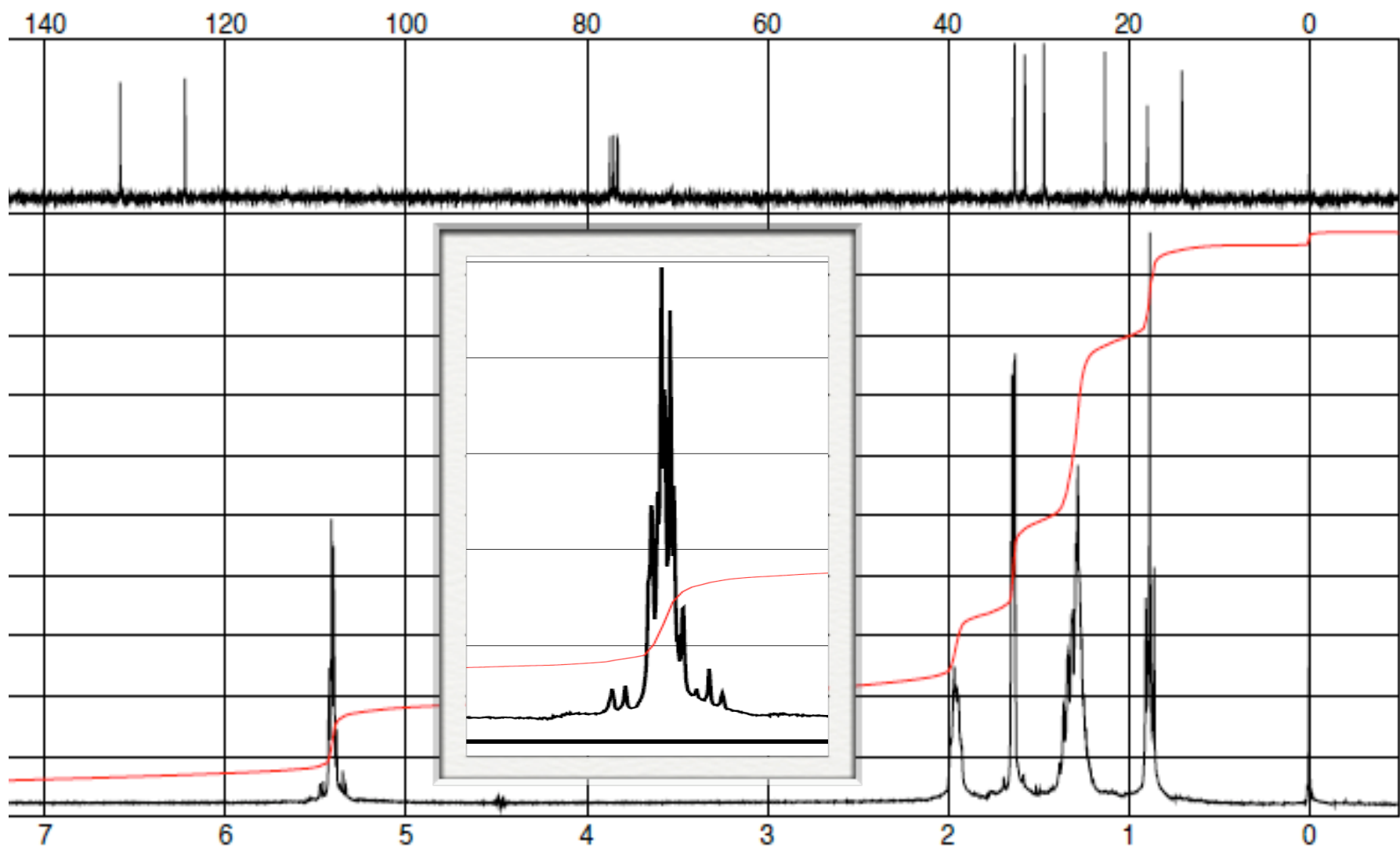
C-H変角振動 (trans alkenes)



3193	86	2733	84	1266	81	758	81
2959	4	2670	85	1207	85	740	81
2941	14	1455	42	1098	79		
2926	9	1456	42	1060	70		
2875	15	1439	55	987	25		
2864	20	1379	59	892	81		
2844	28	1340	74	886	81		

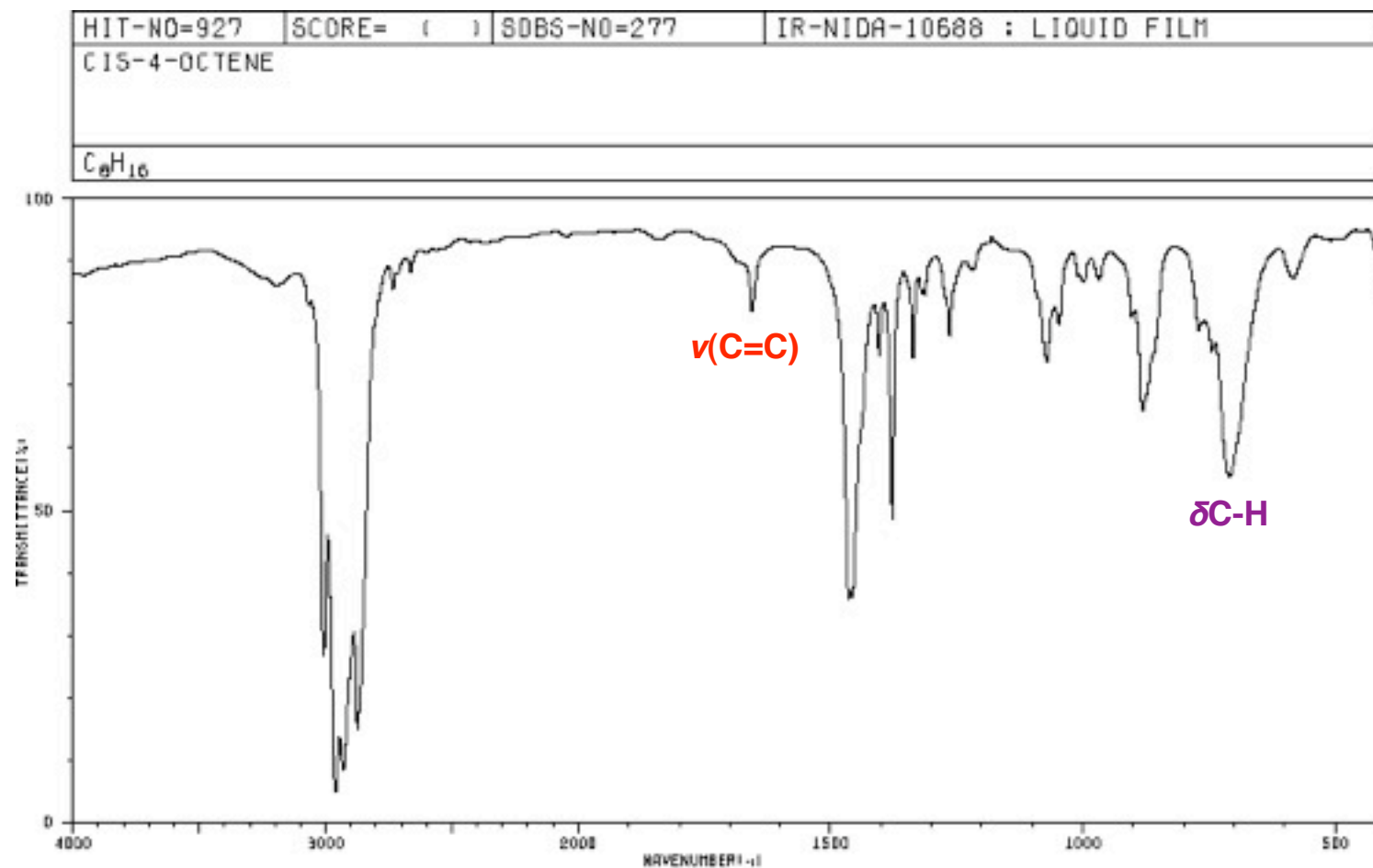






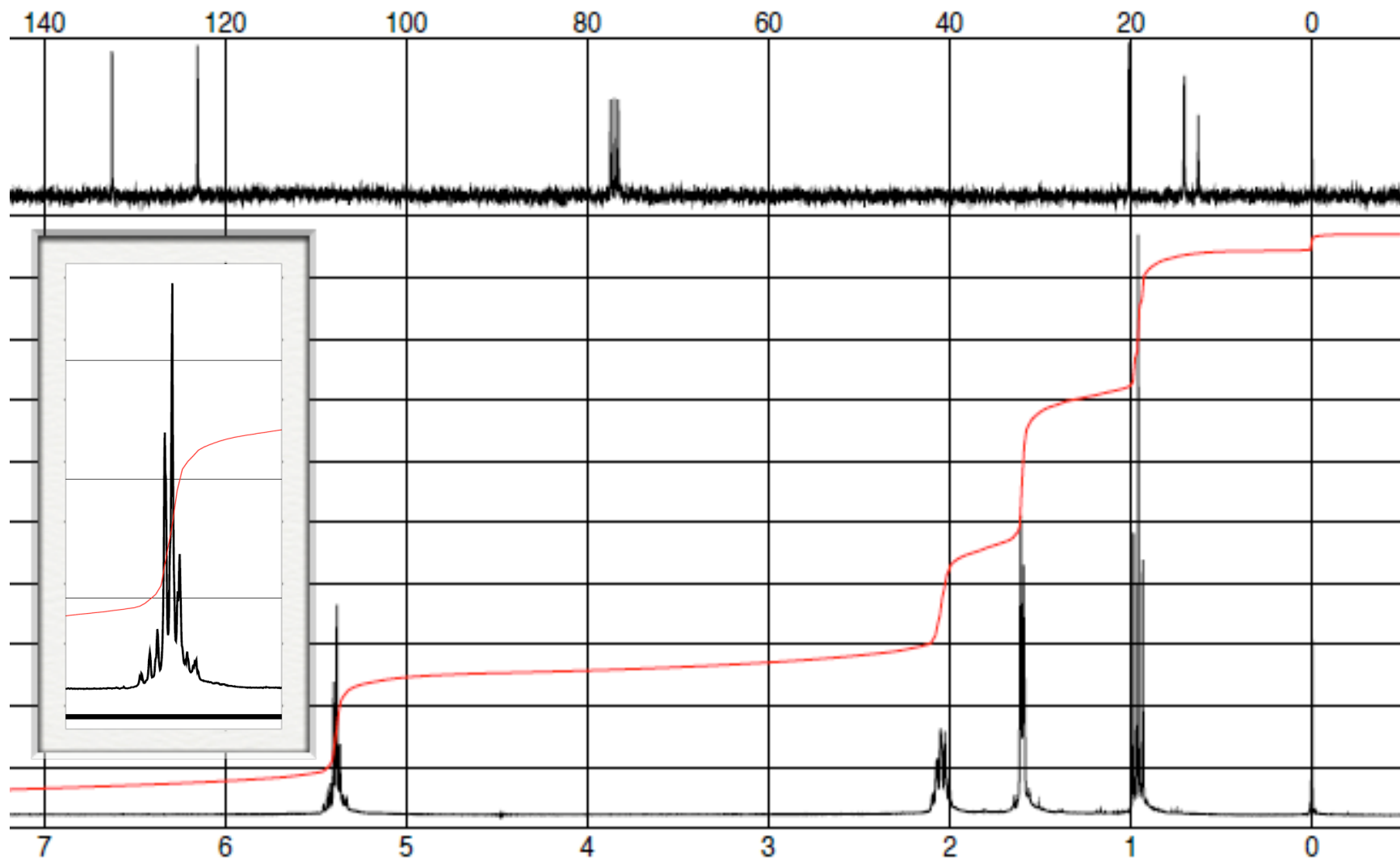


C-H変角振動 (cis alkenes)

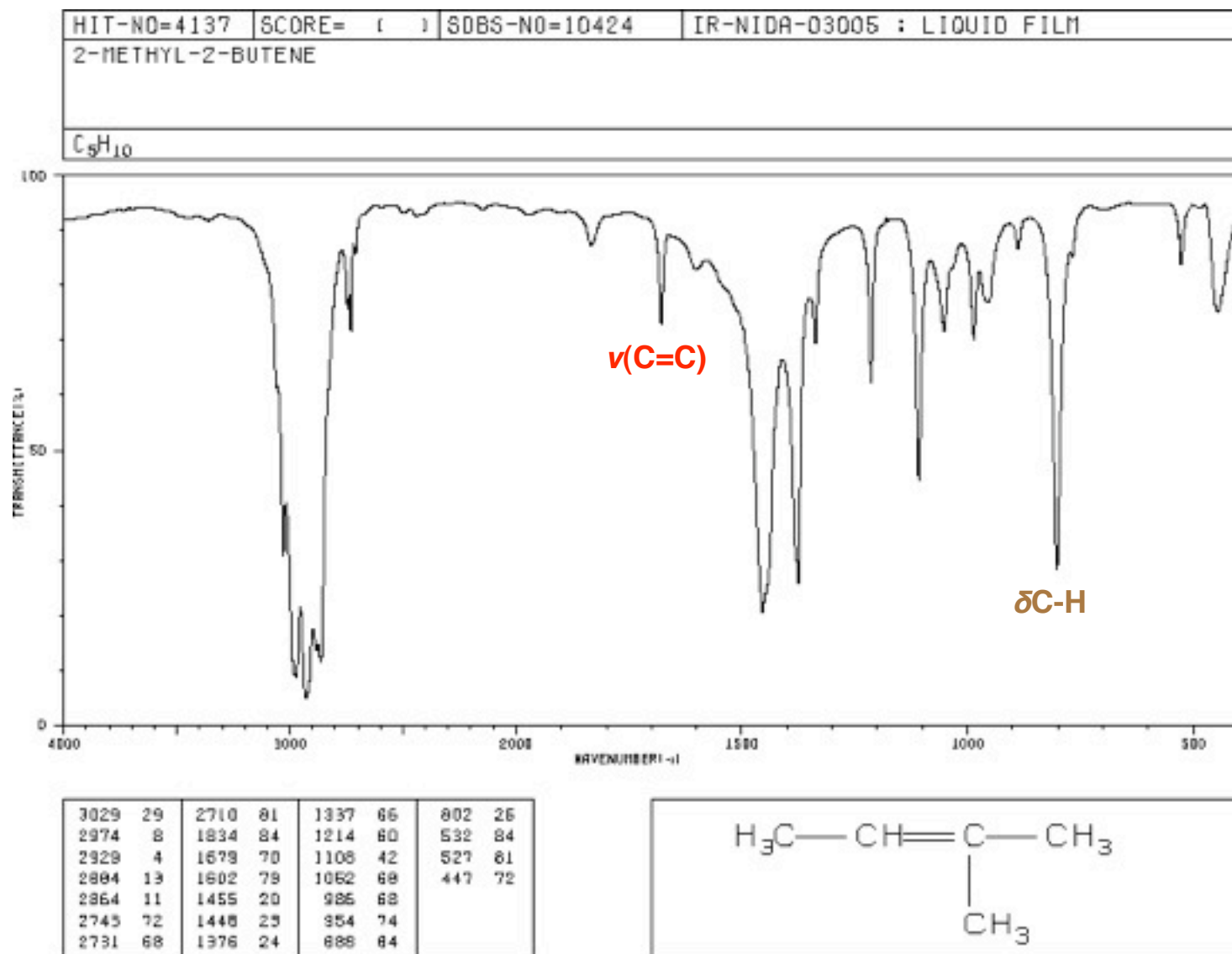


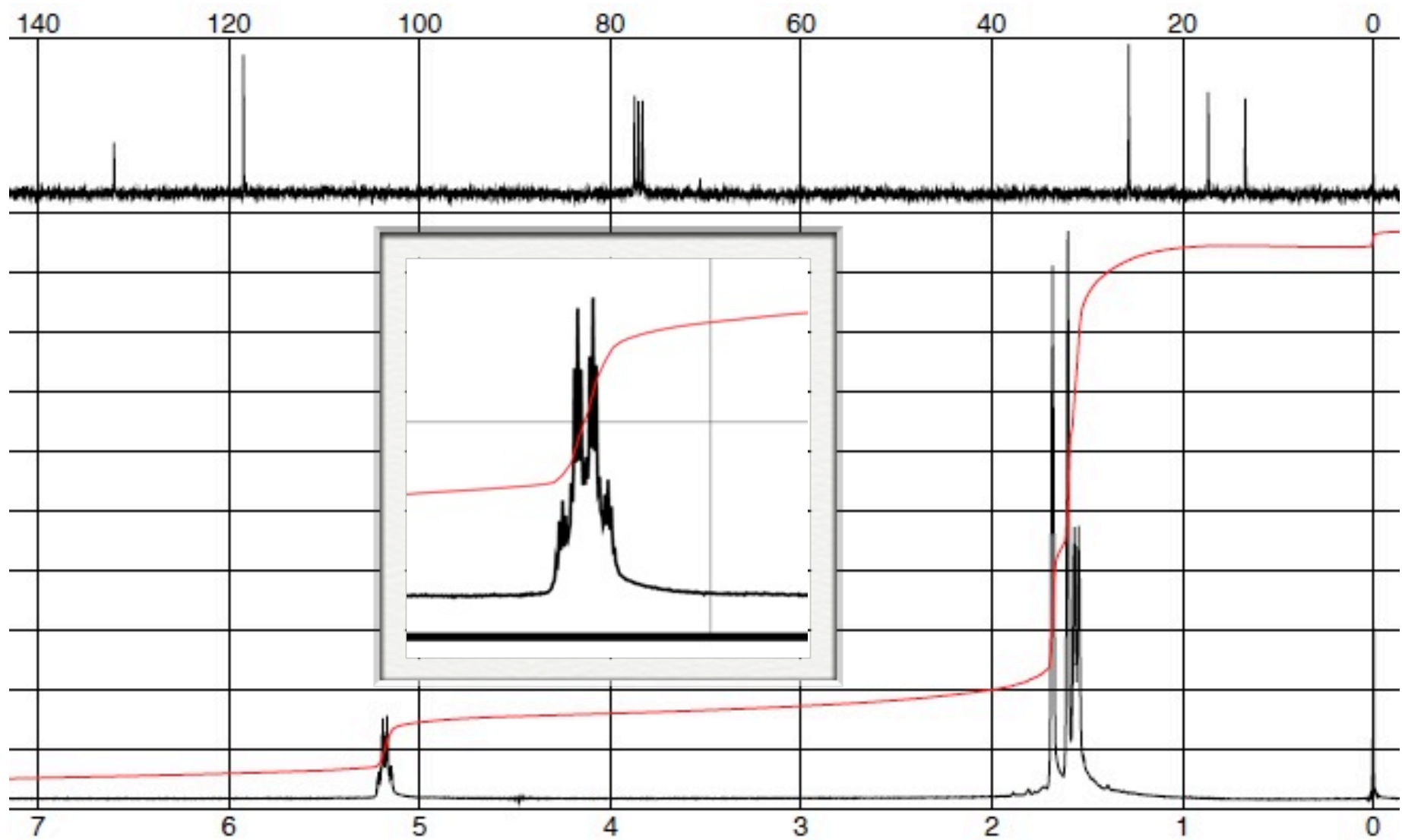
3190	84	2653	84	1320	81	1010	84	745	72
3007	26	1655	79	1313	81	1002	84	710	53
2959	4	1465	34	1264	74	997	84	565	54
2931	7	1457	36	1216	84	966	84		
2874	14	1404	72	1072	70	883	54		
2733	81	1378	46	1061	79	875	56		
2714	84	1337	72	1047	77	772	77		

$$\text{CH}_3 - (\text{CH}_2)_2 - \underset{\text{H}}{\text{C}} = \underset{\text{H}}{\text{C}} - (\text{CH}_2)_2 - \text{CH}_3$$



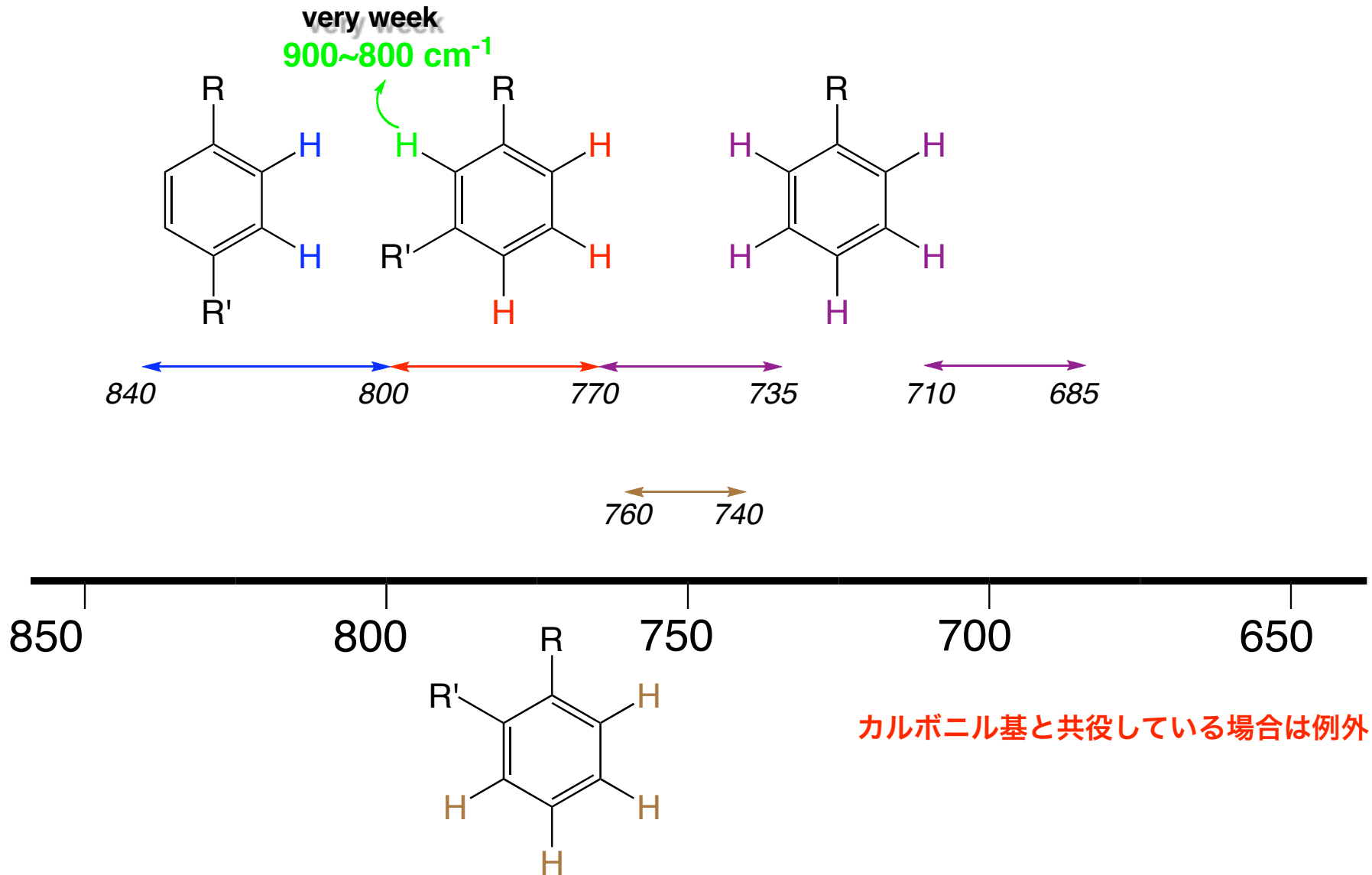
C-H変角振動 (tri-substituted alkenes)



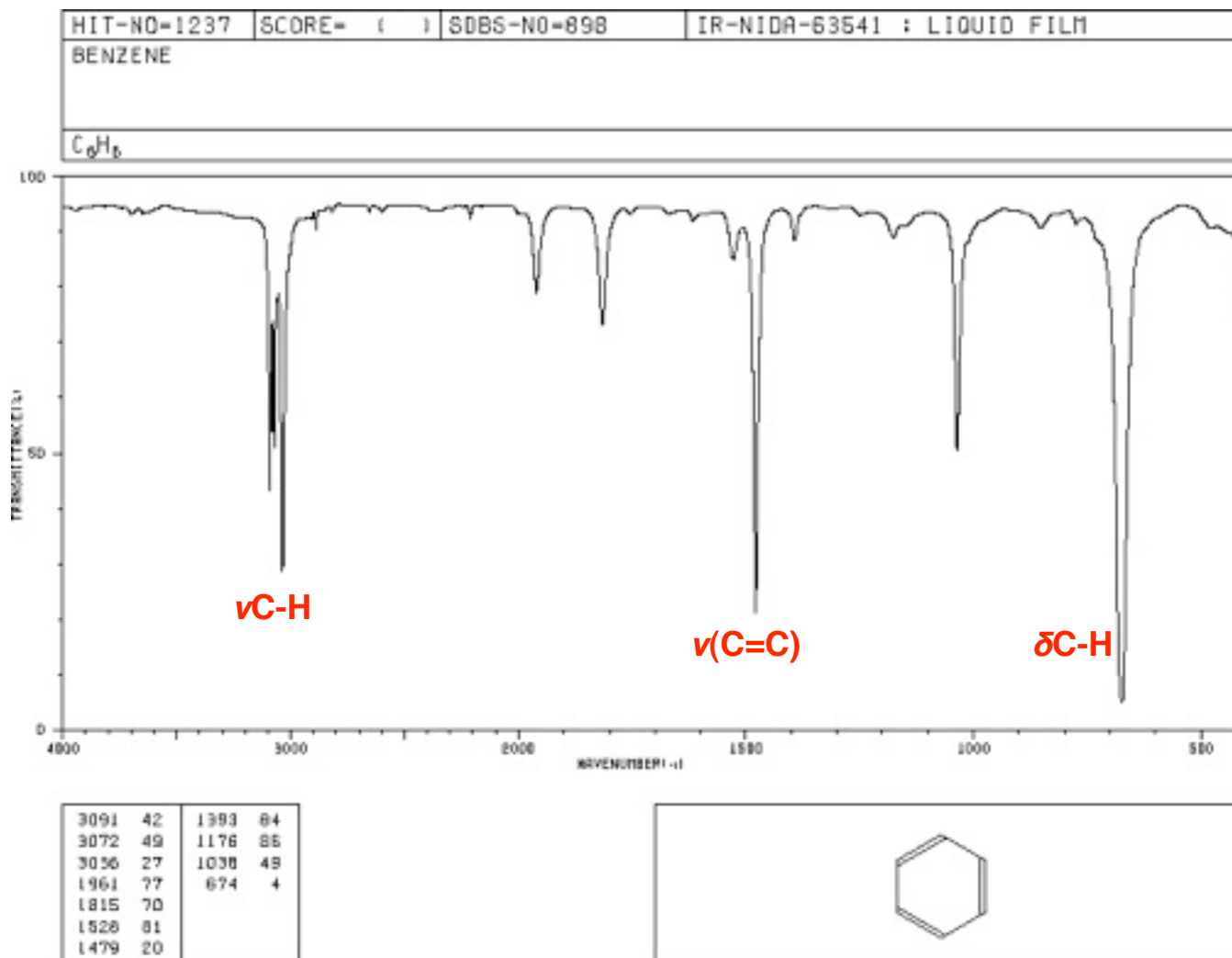


置換パターンに関する情報 (2)

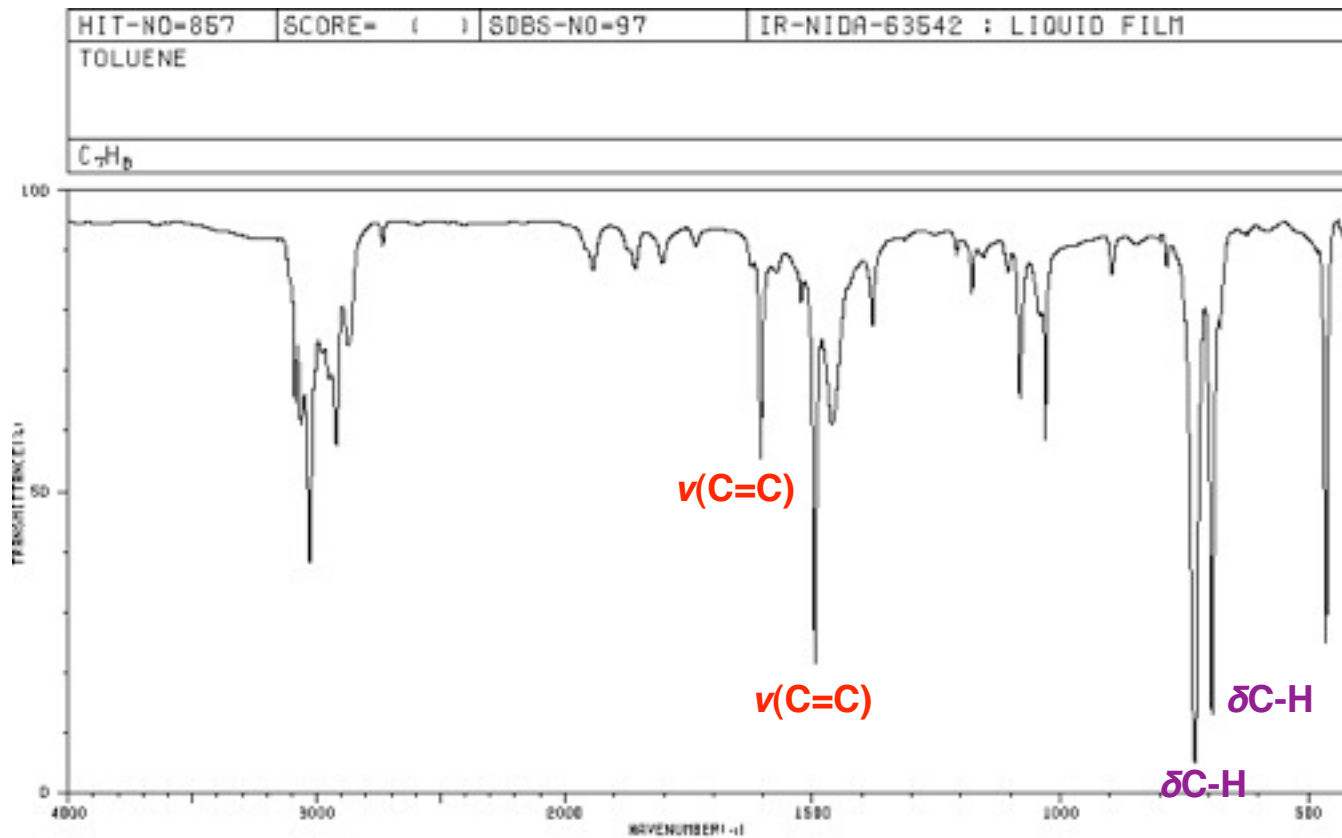
(ベンゼン誘導体)



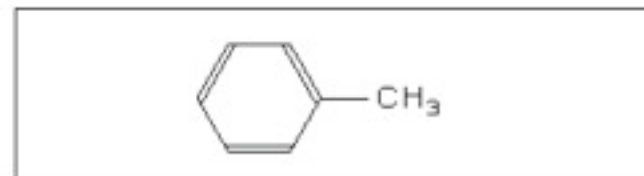
C-H変角振動 (benzene)



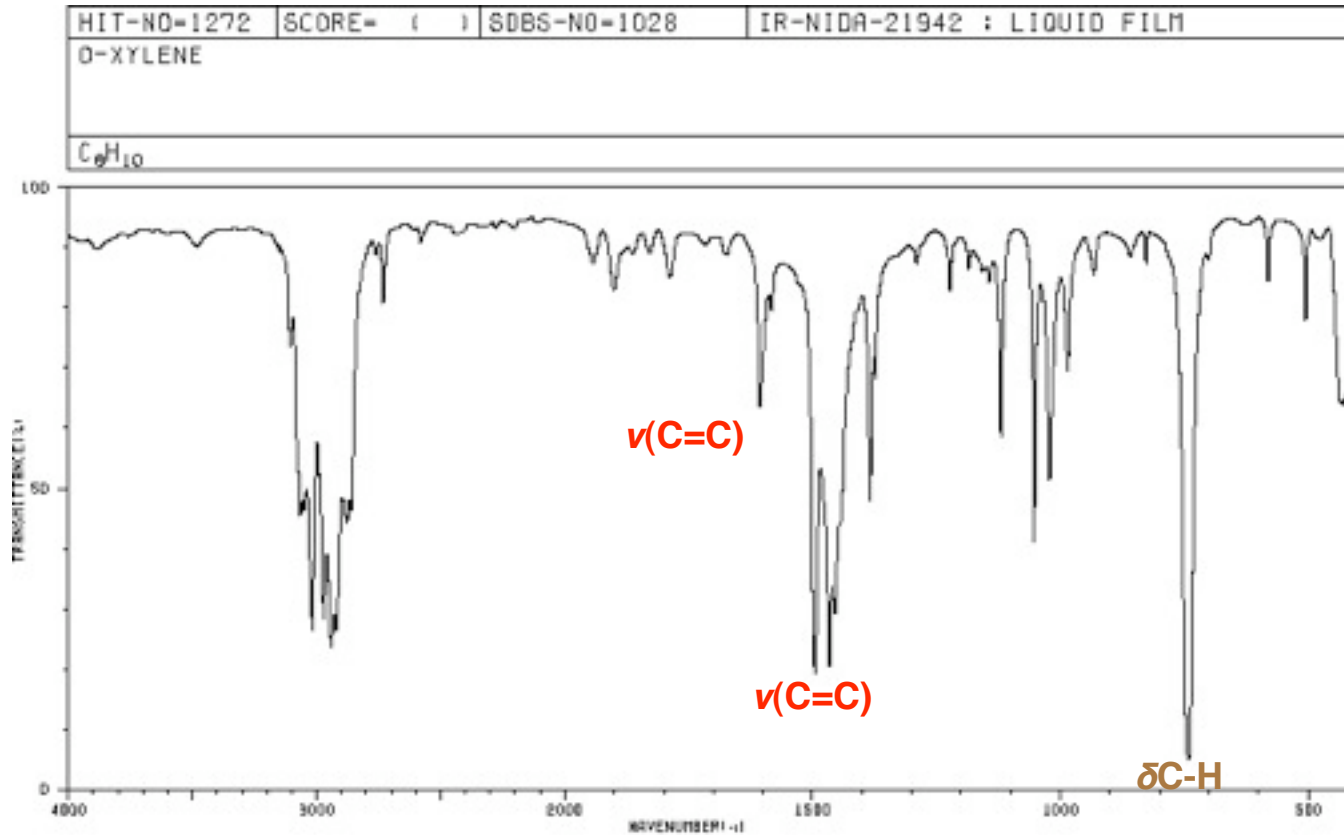
C-H変角振動 (monosubstituted benzene)



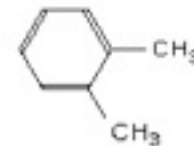
3087	62	1658	84	1210	86	896	81
3062	58	1603	84	1179	79	786	84
3020	37	1605	55	1156	86	729	4
2948	66	1624	79	1107	84	696	12
2920	55	1496	20	1082	62	678	74
2873	70	1461	58	1042	77	465	25
1942	84	1379	74	1030	67		



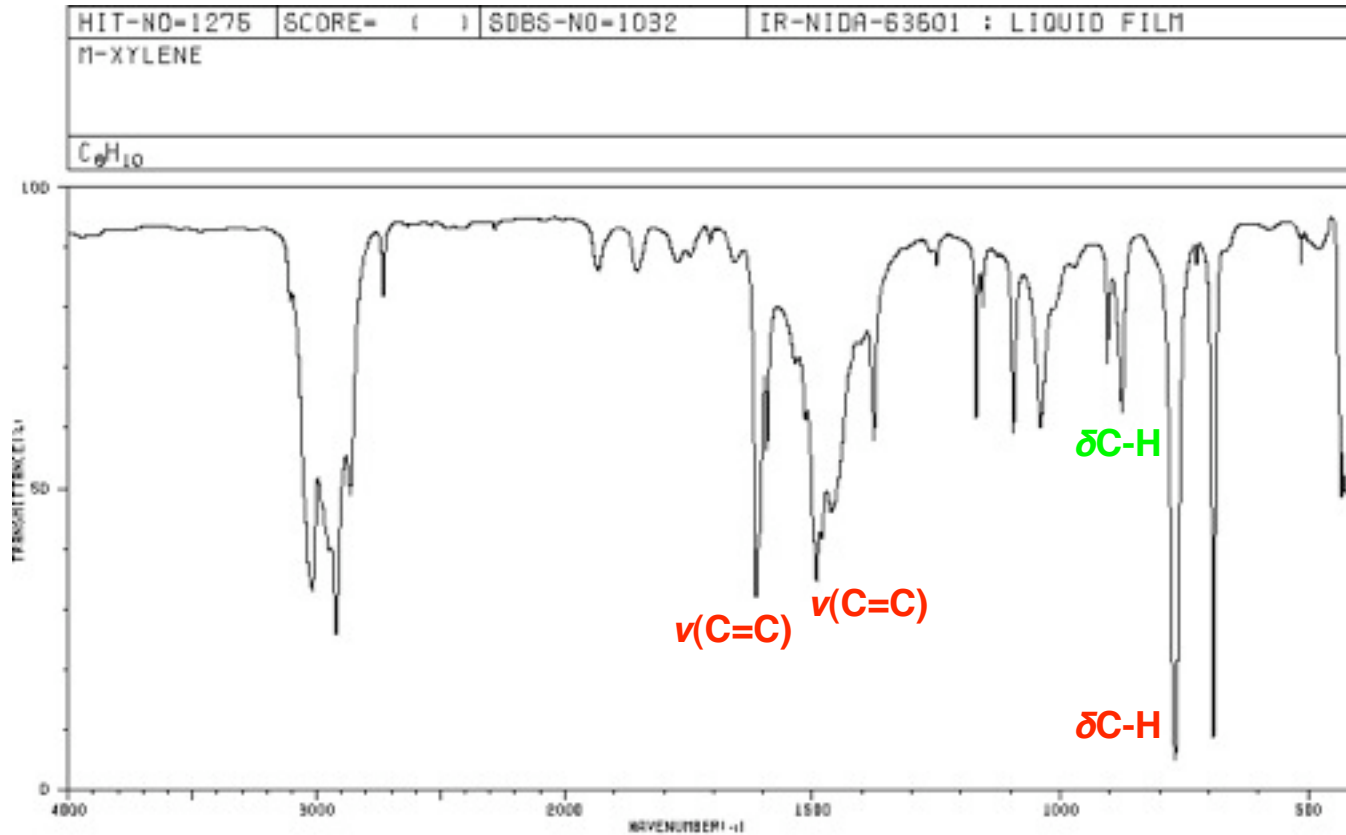
C-H変角振動 (ortho-disubstituted benzene)



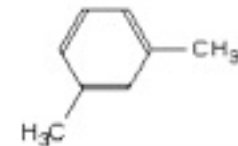
3108	70	2878	42	1689	77	1223	79	986	66
3066	43	2860	44	1495	18	1186	84	932	81
3050	44	2732	77	1467	20	1157	81	742	4
3018	26	1942	84	1466	27	1146	81	682	81
2971	26	1901	79	1384	46	1120	57	506	74
2940	22	1787	81	1374	86	1053	39	436	62
2921	26	1606	60	1291	84	1022	49	431	62



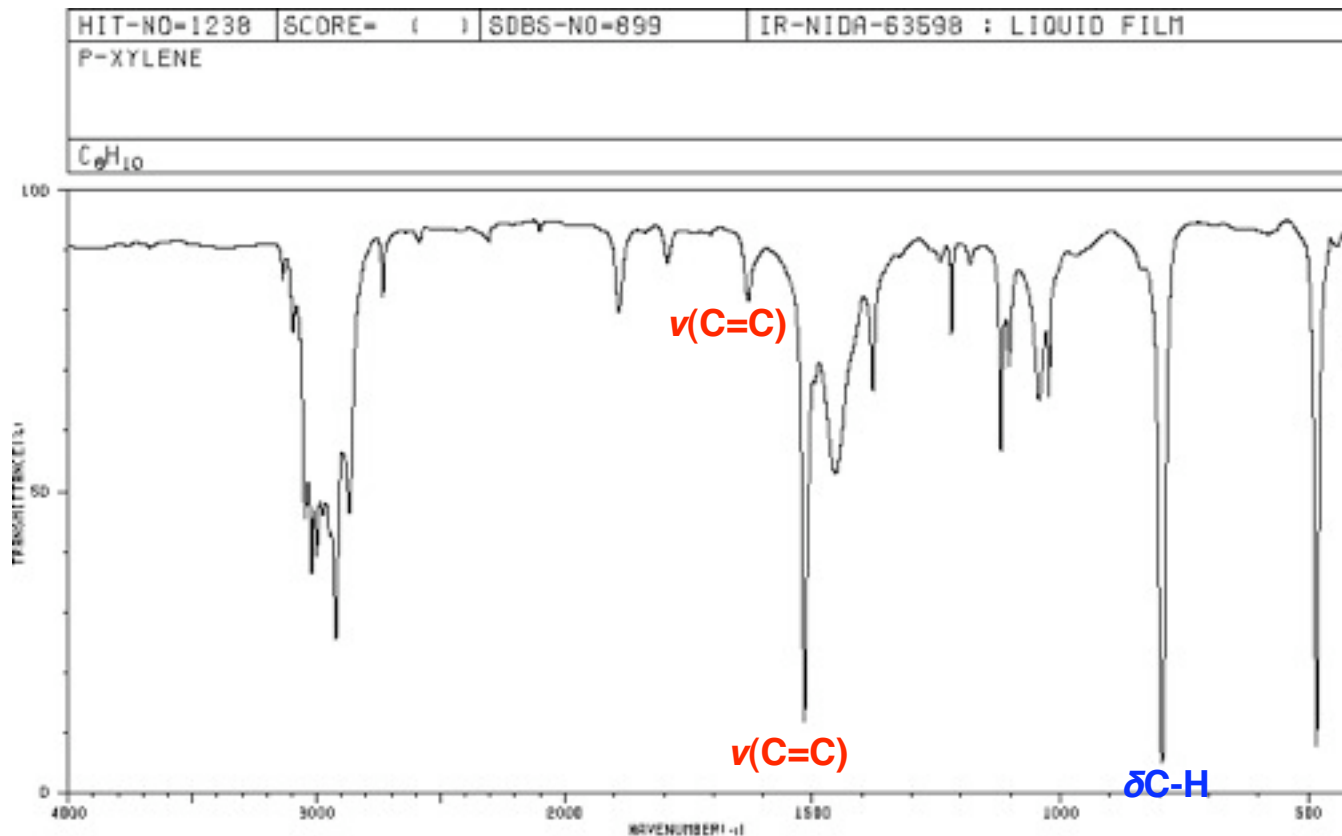
C-H変角振動 (meta-disubstituted benzene)



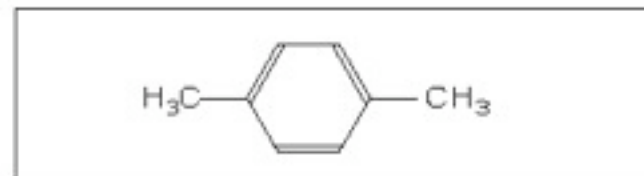
3106	79	1664	84	1492	33	1170	68	726	84
3016	32	1772	84	1482	39	1157	77	691	8
2940	37	1764	84	1462	44	1085	57	515	84
2921	24	1668	84	1376	66	1040	67	493	86
2864	47	1614	31	1263	86	905	68	478	86
2732	79	1592	55	1256	86	876	60	434	46
1932	84	1616	68	1250	84	769	4		



C-H変角振動 (para-disubstituted benzene)

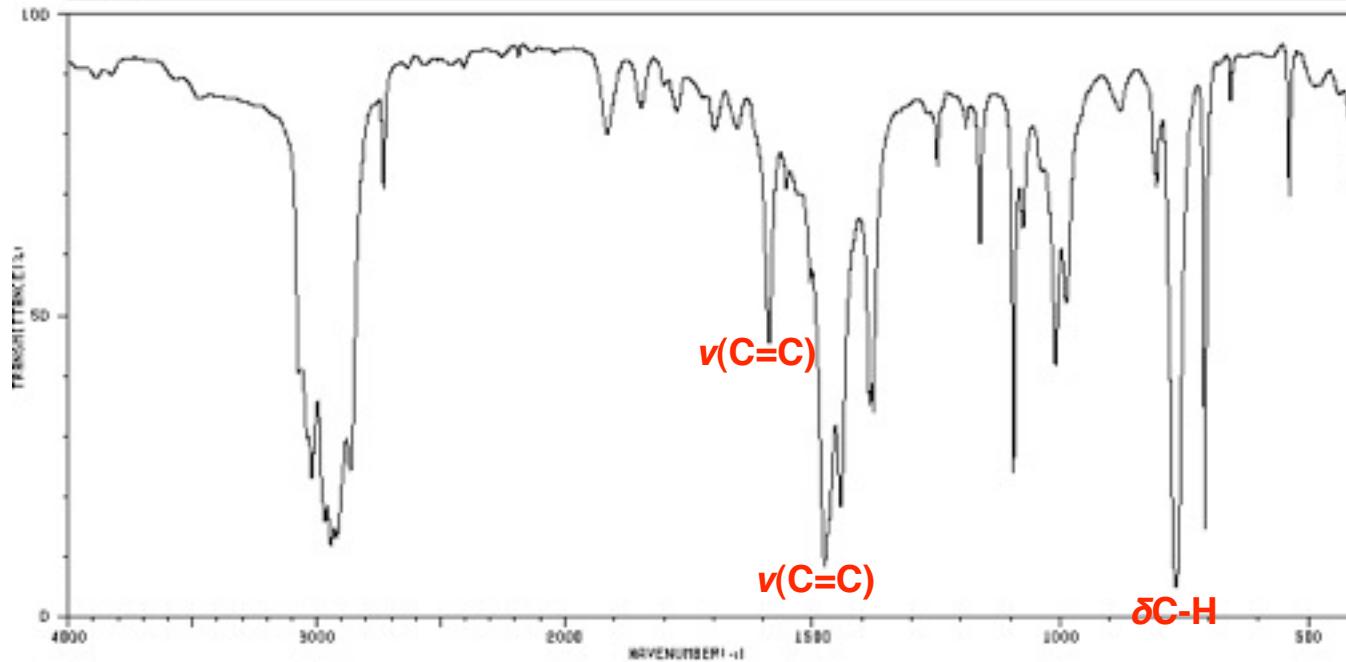


3136	81	2923	24	1464	60	1043	62
3095	74	2868	44	1378	64	1023	64
3047	43	2733	79	1243	84	785	4
3020	36	1690	77	1220	72	484	7
3000	37	1793	84	1183	84		
2976	44	1630	79	1120	55		
2946	41	1616	11	1103	68		



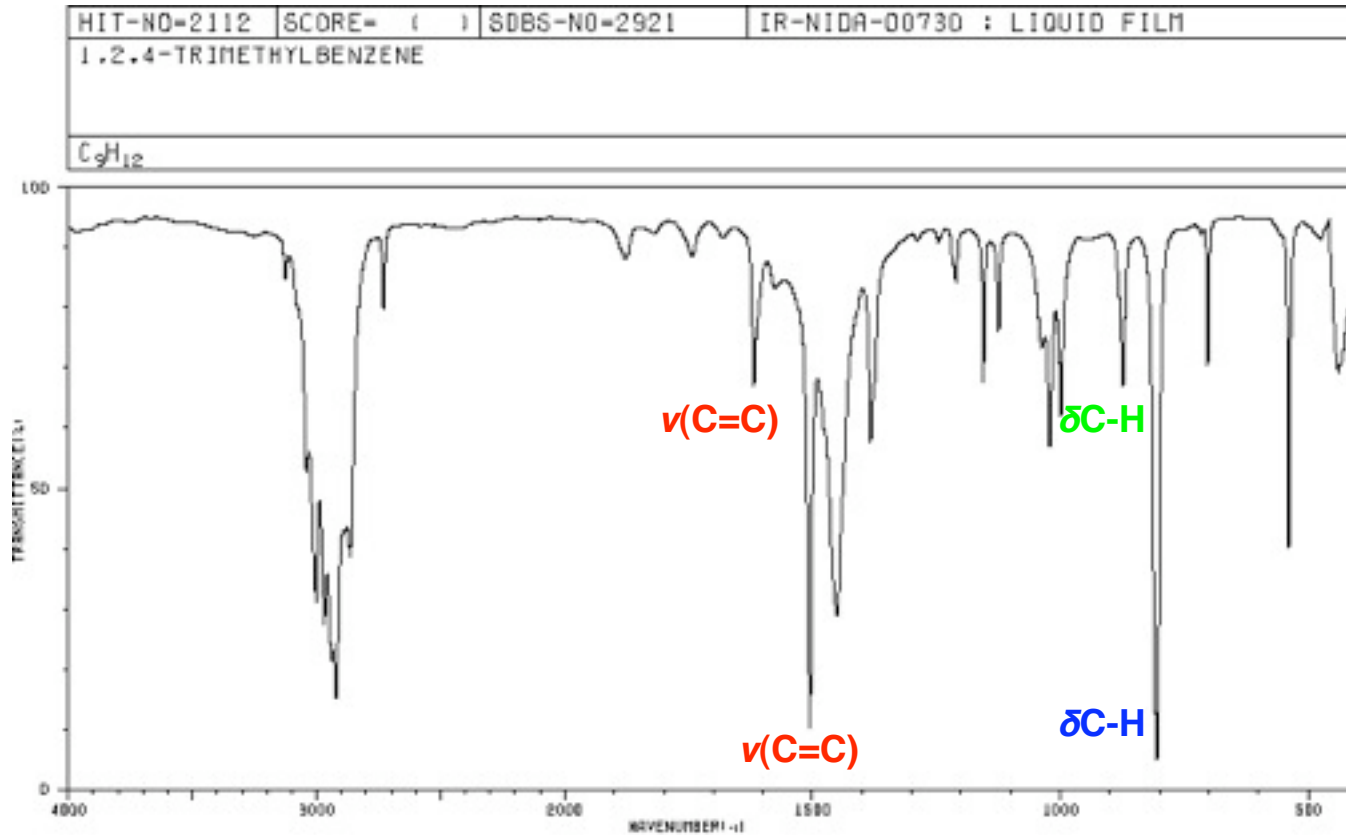
C-H変角振動 (1,2,3-trisubstituted benzene)

HIT-NO=1245	SCORE= ()	SDBS-NO=906	IR-NIDA-64857 : LIQUID FILM
1,2,3-TRIMETHYLBENZENE			
C ₉ H ₁₂			

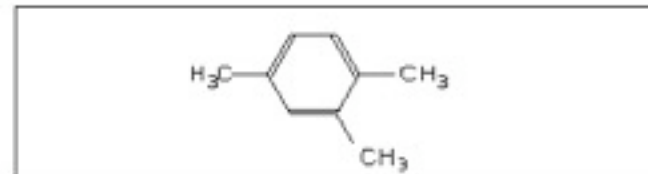


3038	28	1914	77	1606	63	1153	68	807	68
3019	21	1845	81	1476	8	1094	23	767	4
2966	15	1773	81	1443	17	1076	62	709	13
2942	11	1698	77	1386	34	1010	39	667	81
2919	12	1652	79	1378	33	988	50	538	66
2864	23	1588	43	1249	72	879	81	485	84
2730	68	1563	68	1191	79	813	74	480	84

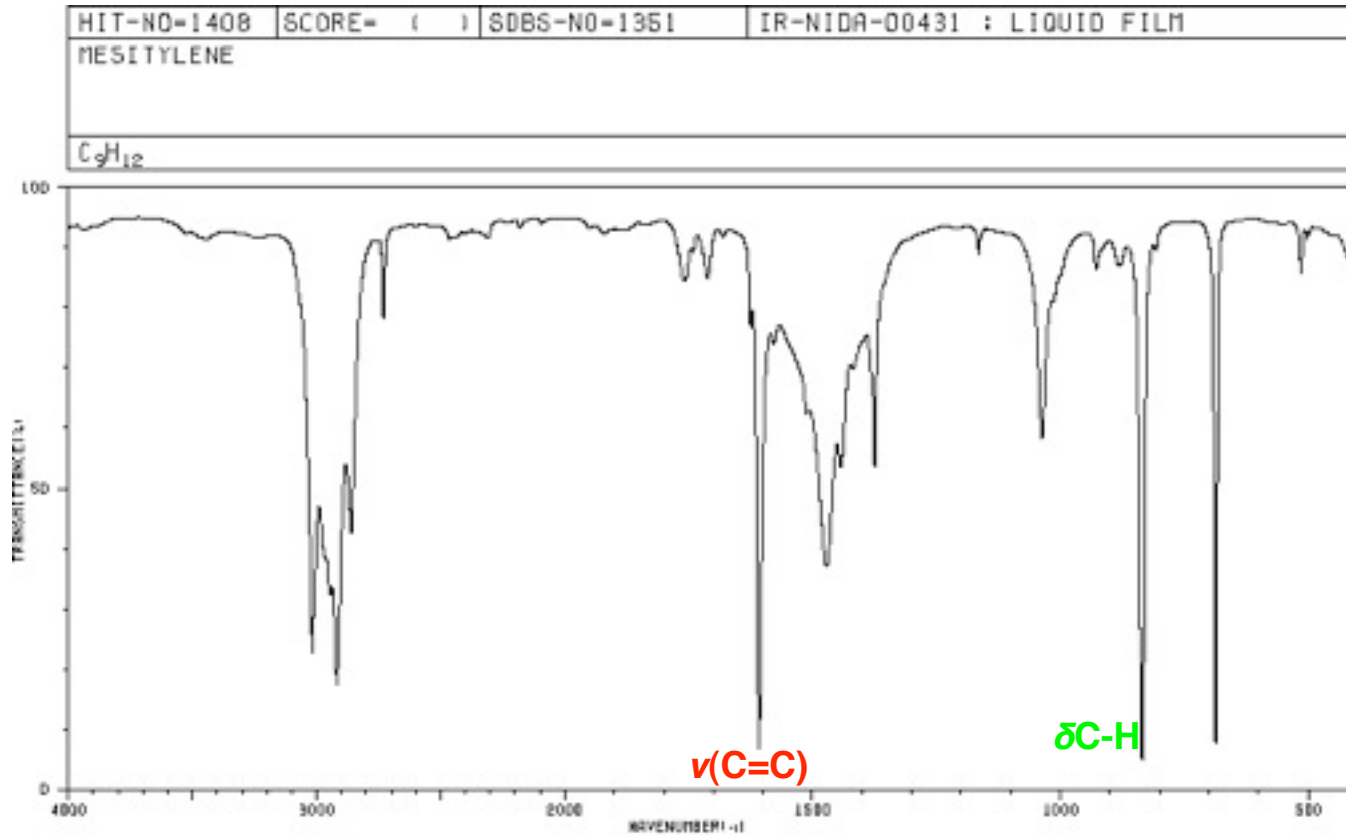
C-H変角振動 (1,2,4-trisubstituted benzene)



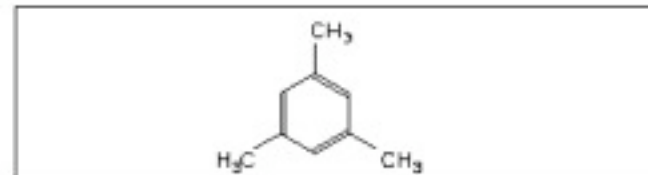
3126	81	2730	77	1383	66	999	60
3041	50	1877	84	1217	84	874	64
3002	30	1743	84	1211	81	806	4
2970	26	1619	84	1166	64	703	68
2939	20	1576	79	1125	72	539	39
2922	14	1505	10	1030	70	440	66
2864	37	1461	27	1021	66		

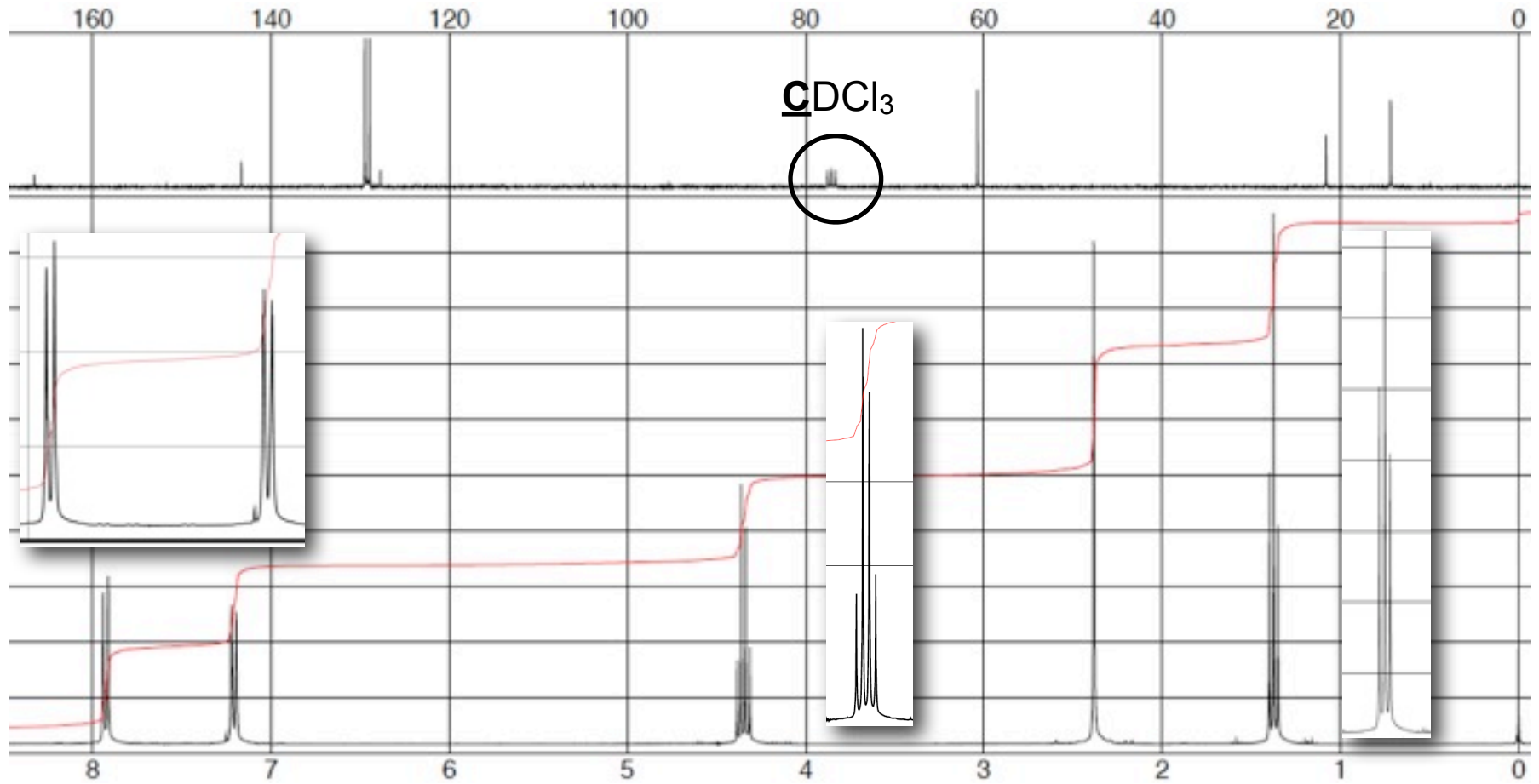


C-H変角振動 (1,3,5-trisubstituted benzene)

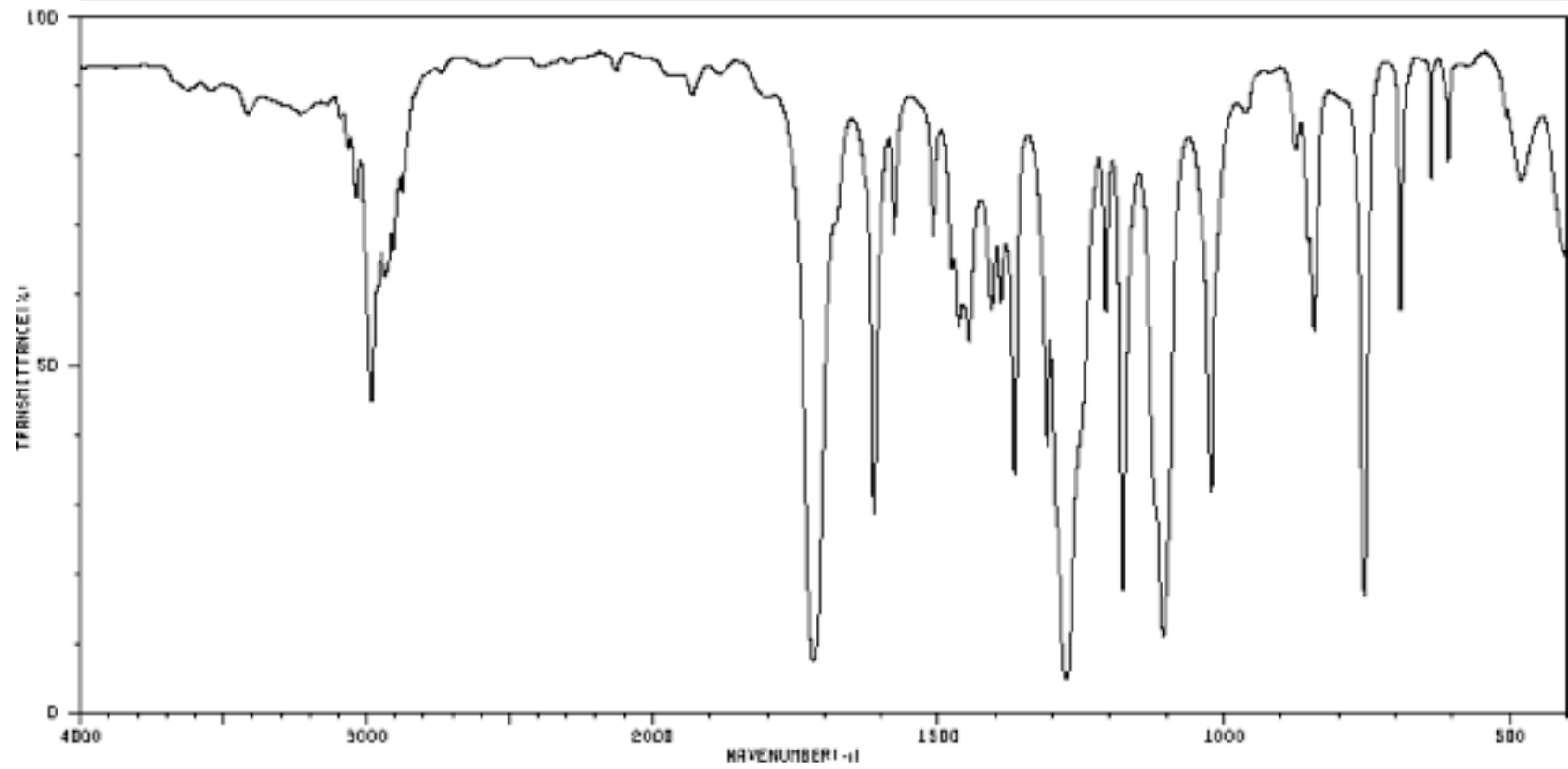


3017	21	1626	74	1037	66
2945	31	1609	6	929	84
2910	16	1570	70	801	84
2861	41	1472	36	696	4
2731	74	1443	52	688	7
1759	81	1375	52	515	81
1712	81	1166	86		



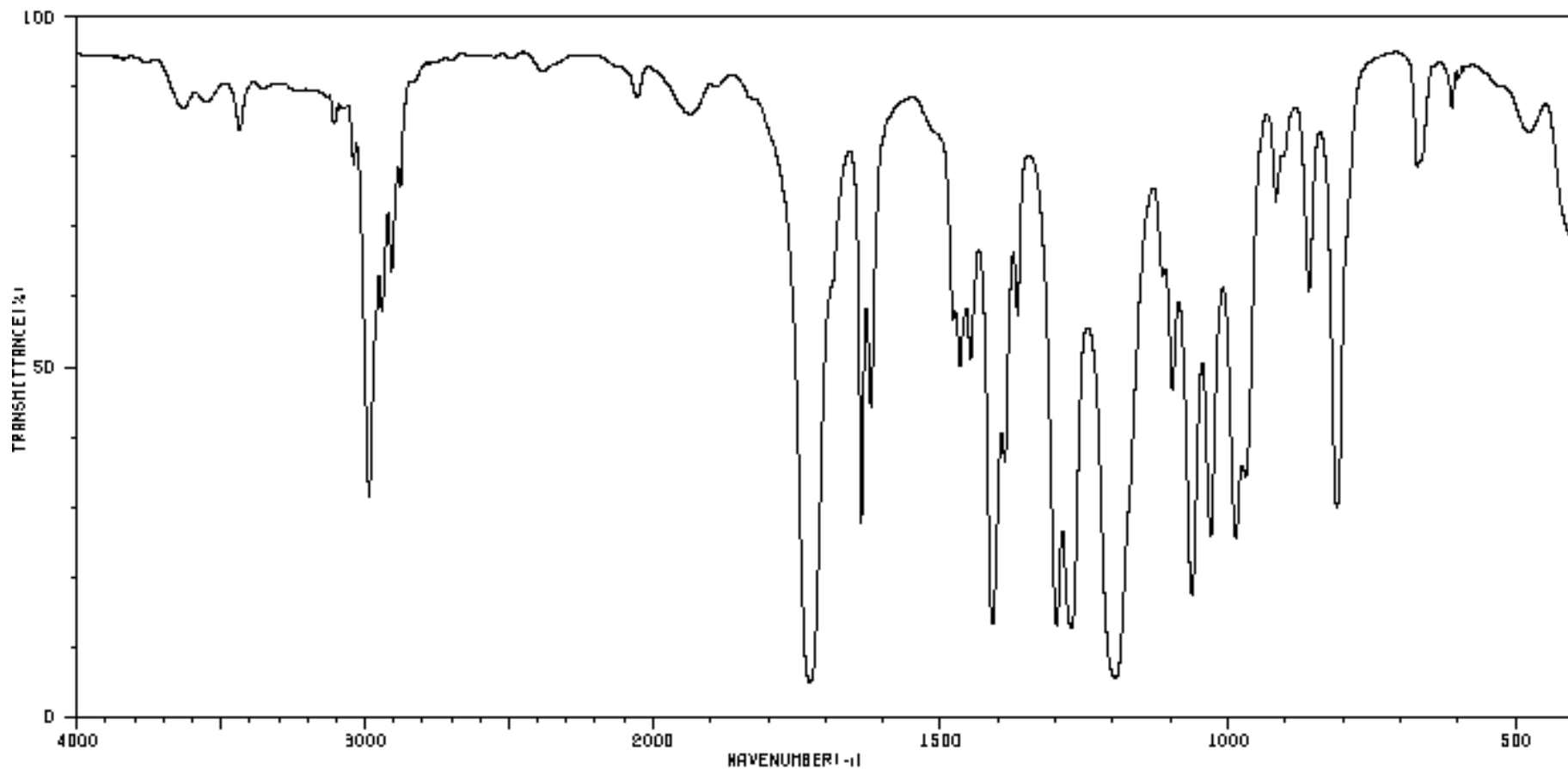


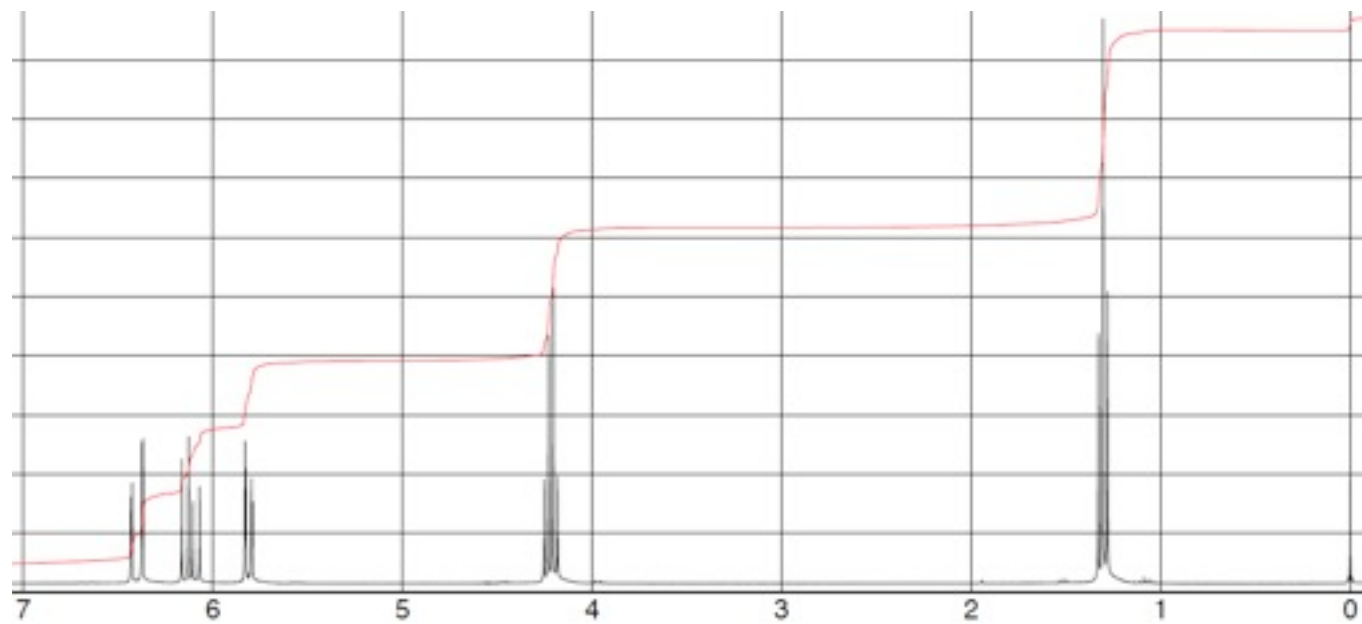
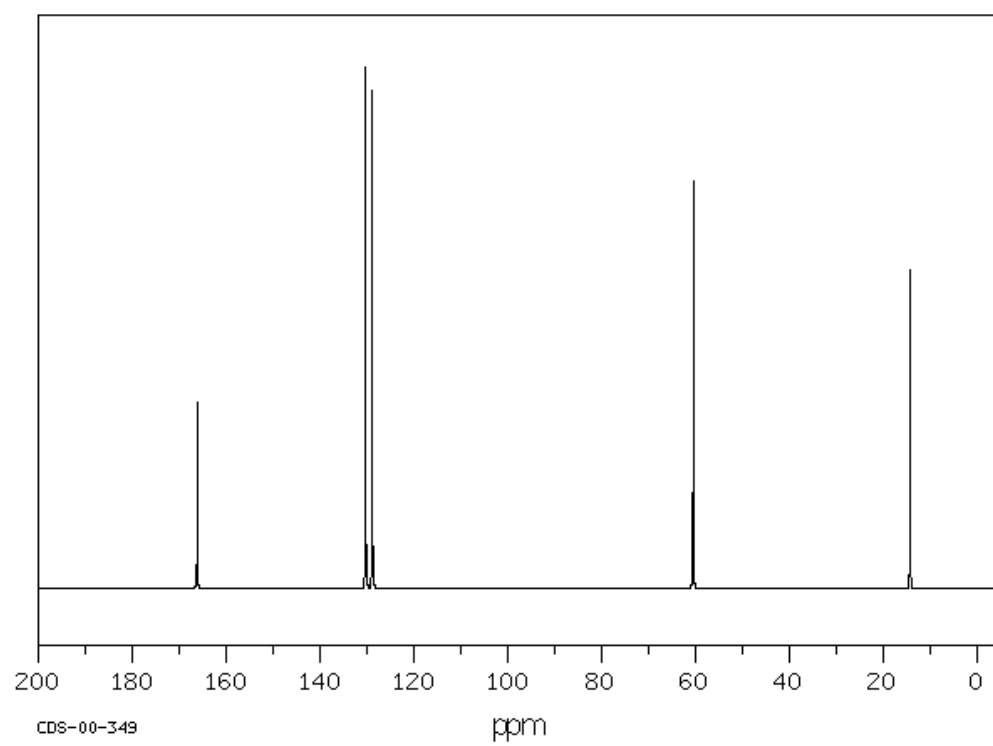
LIQUID FILM



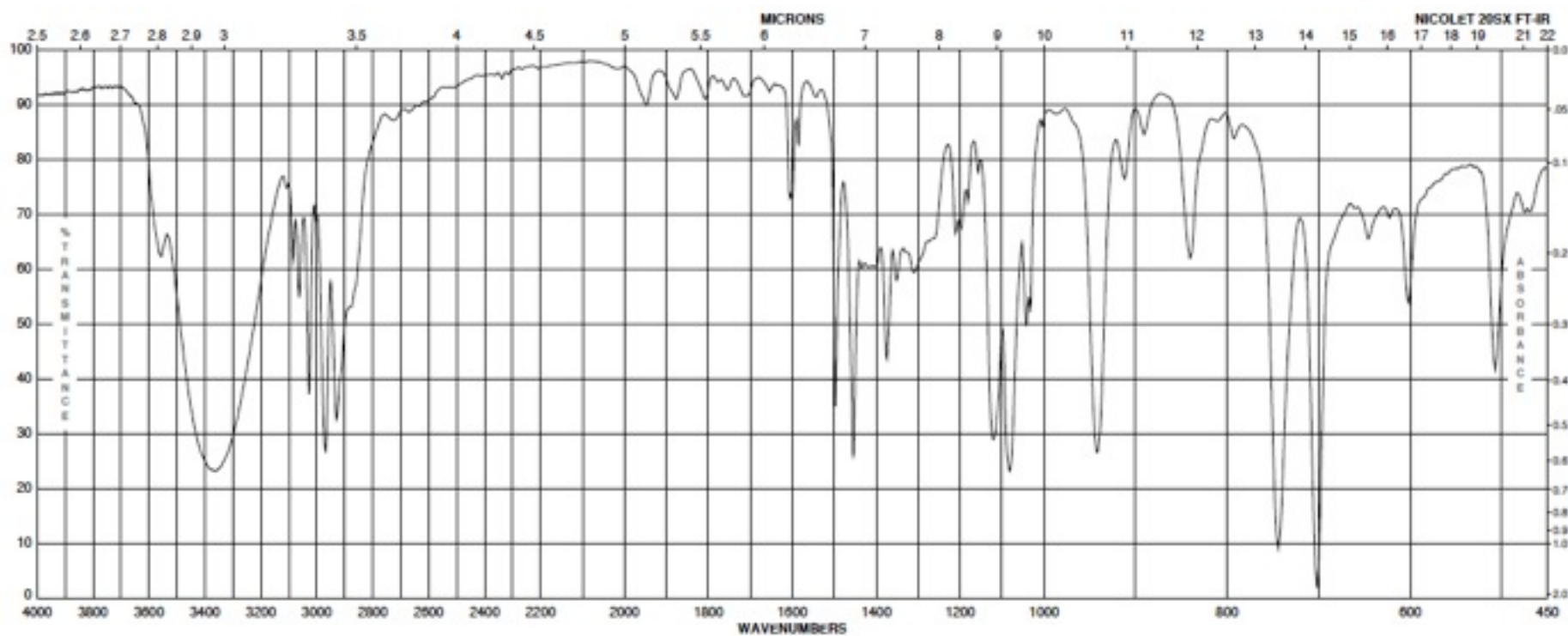
3417	81	2907	64	1464	63	1276	4	863	66
3228	84	2874	72	1458	57	1208	55	842	52
3064	77	1719	7	1447	50	1178	17	755	16
3036	72	1613	27	1407	56	1107	10	692	56
2982	43	1578	66	1391	57	1022	30	638	74
2961	56	1510	65	1367	33	962	64	608	77
2936	60	1478	62	1310	36	874	77	480	74

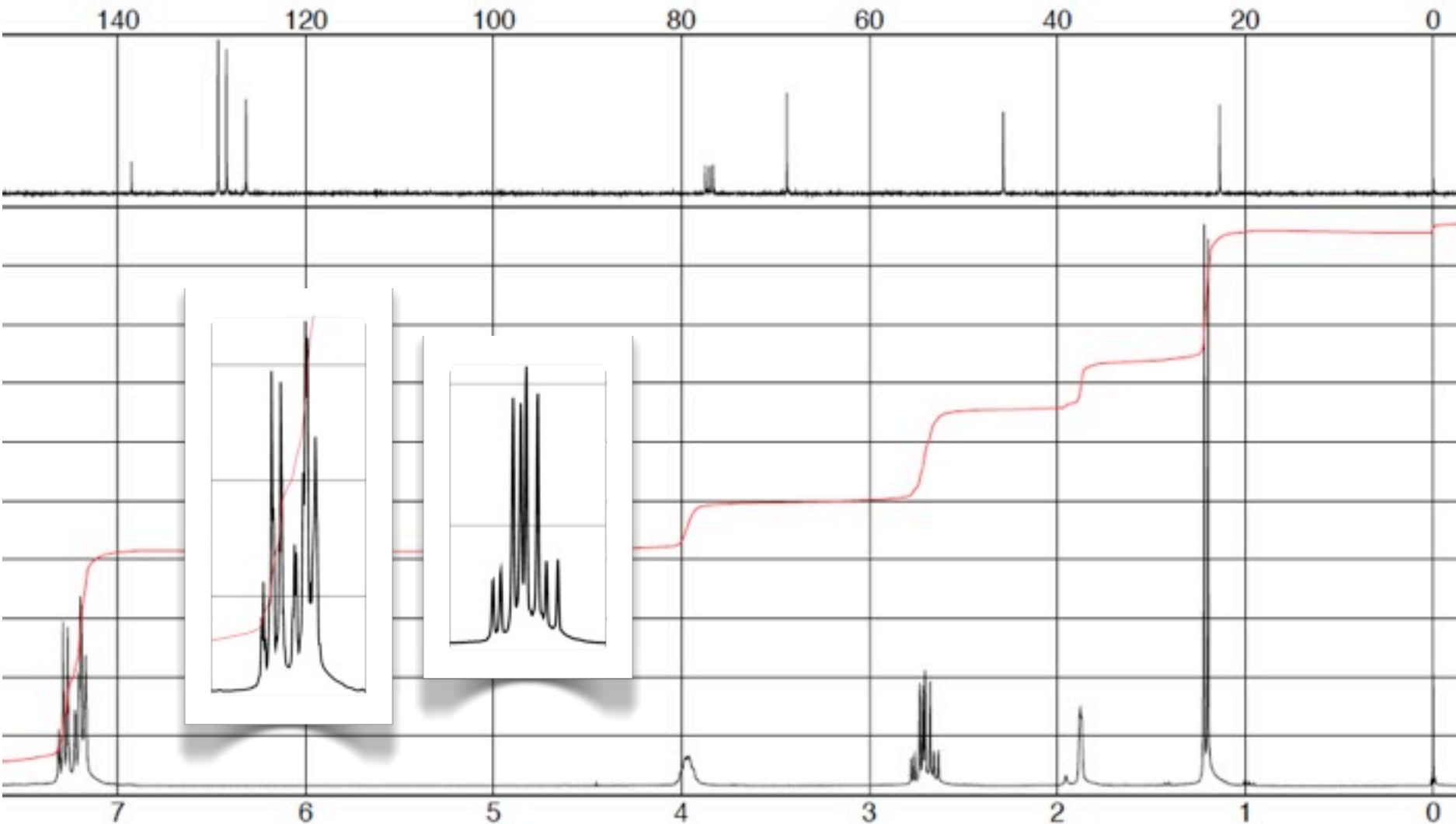
次のIR, ^1H NMR, ^{13}C NMRスペクトルから、
化合物の構造を推定しなさい。



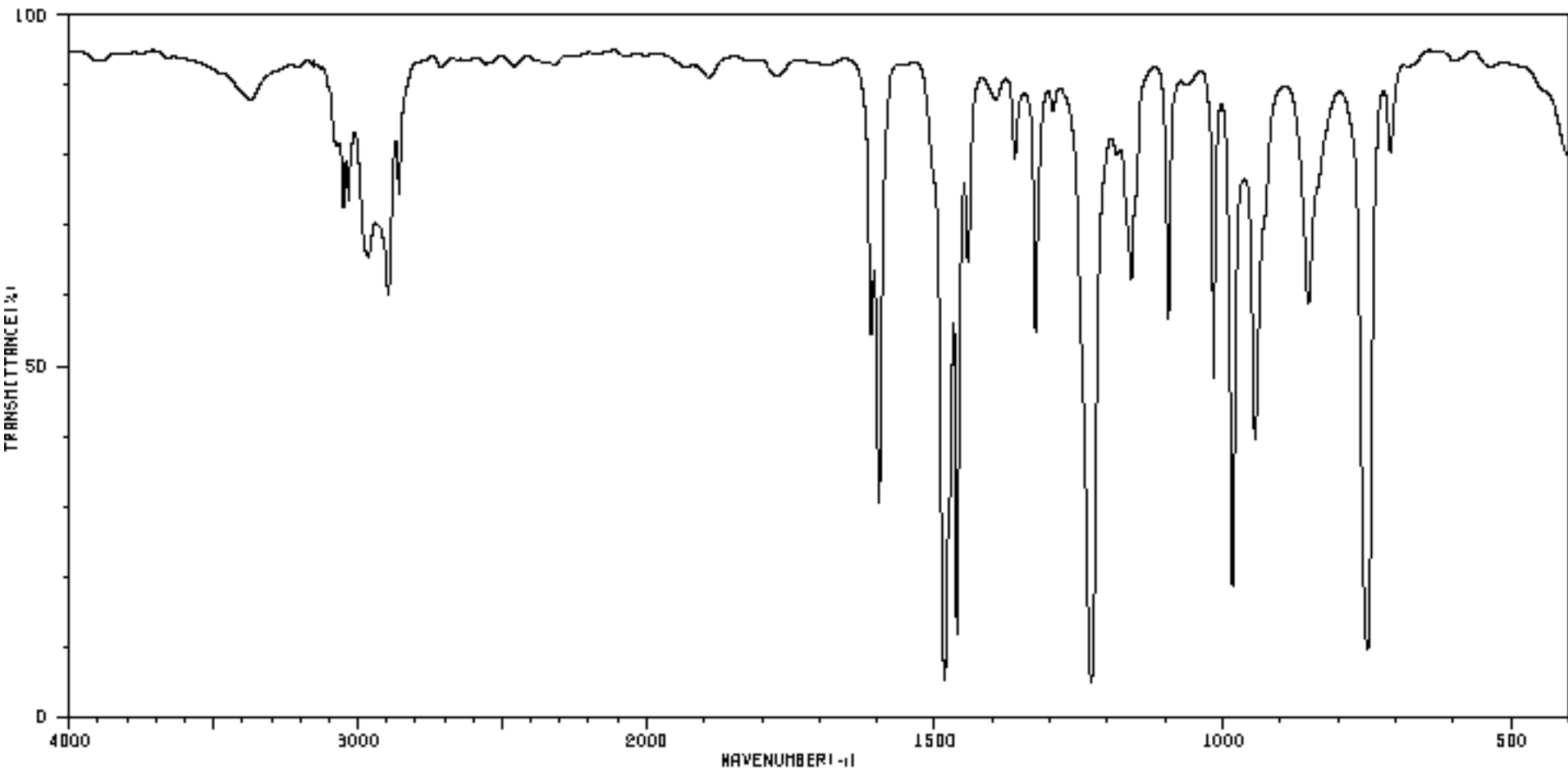


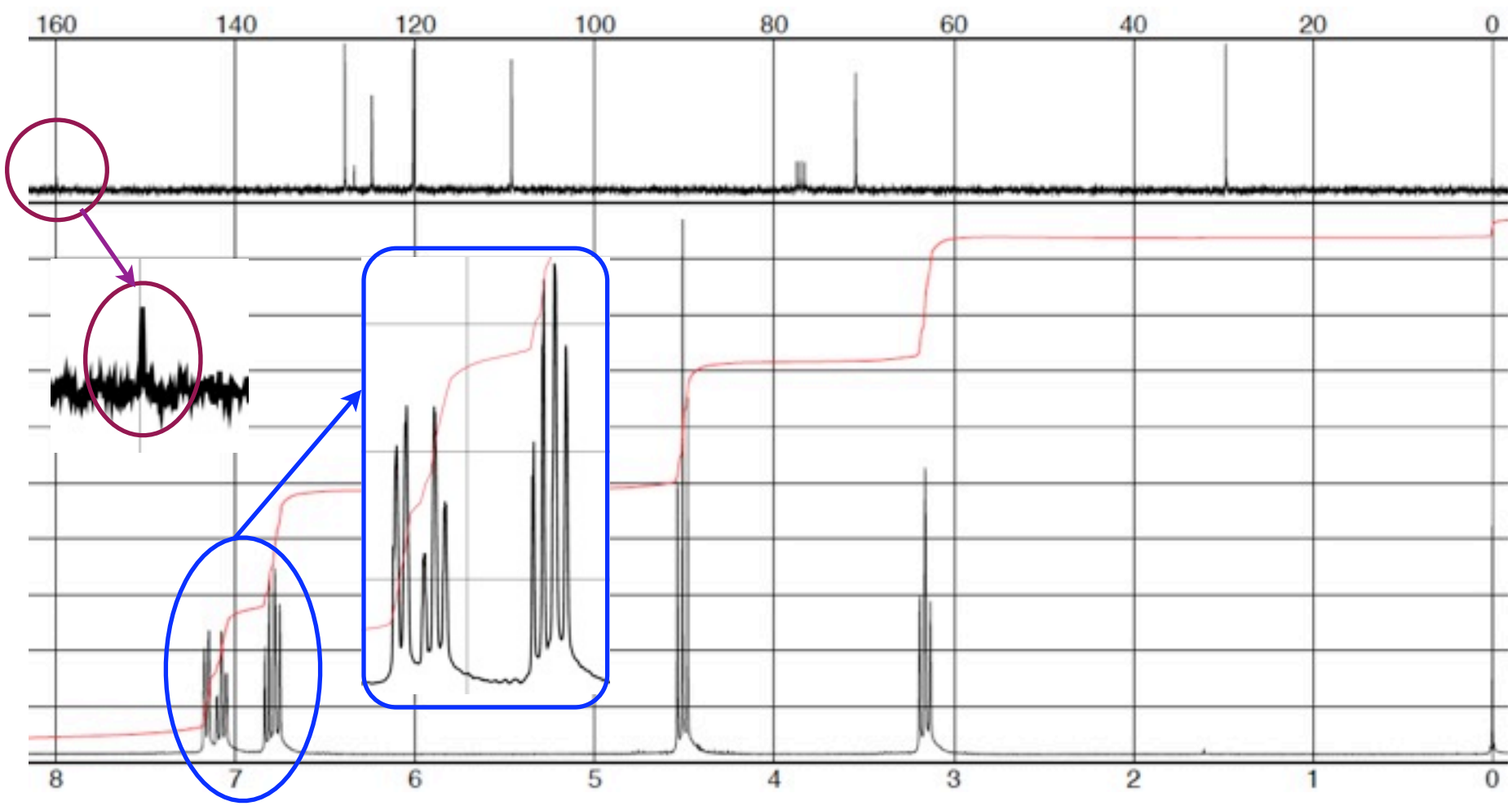
次のIR, ^1H NMR, ^{13}C NMRスペクトルから、
化合物の構造を推定しなさい。





次のIR, ^1H NMR, ^{13}C NMRスペクトルから、
化合物 ($\text{C}_8\text{H}_8\text{O}$) の構造を推定しなさい。





次のIR, ^1H NMR, ^{13}C NMRスペクトルから、
窒素原子を1個含む化合物の構造を推定しなさい。

