

Spectroscopy

Infrared Spectra

III Pharm .D

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Infrared spectra in this presentation are taken by permission from the SDBS web site:

SDBSWeb: <http://www.aist.go.jp/RIODB/SDBS/>



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Spectroscopy

“seeing the unseeable”

Using electromagnetic radiation as a probe to obtain information about atoms and molecules that are too small to see.

Electromagnetic radiation is propagated at the speed of light through a vacuum as an oscillating wave.

electromagnetic relationships:

$$\lambda \nu = c$$

$$\lambda \propto 1/\nu$$

$$E = h\nu$$

$$E \propto \nu$$

$$E = hc/\lambda$$

$$E \propto 1/\lambda$$

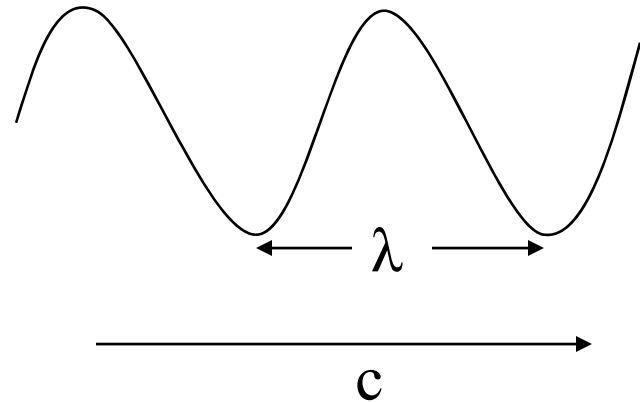
λ = wave length

ν = frequency

c = speed of light

E = kinetic energy

h = Planck's constant



Two oscillators will strongly interact when their energies are equal.

$$E_1 = E_2$$

$$\lambda_1 = \lambda_2$$

$$\nu_1 = \nu_2$$

If the energies are different, they will not strongly interact!

We can use electromagnetic radiation to probe atoms and molecules to find what energies they contain.

some electromagnetic radiation ranges

	<u>Approx. freq. range</u> Hz (cycle/sec)	<u>Approx. wavelengths</u> meters
Radio waves	$10^4 - 10^{12}$	$3 \times 10^4 - 3 \times 10^{-4}$
Infrared (heat)	$10^{11} - 3.8 \times 10^{14}$	$3 \times 10^{-3} - 8 \times 10^{-7}$
Visible light	$3.8 \times 10^{14} - 7.5 \times 10^{14}$	$8 \times 10^{-7} - 4 \times 10^{-7}$
Ultraviolet	$7.5 \times 10^{14} - 3 \times 10^{17}$	$4 \times 10^{-7} - 10^{-9}$
X rays	$3 \times 10^{17} - 3 \times 10^{19}$	$10^{-9} - 10^{-11}$
Gamma rays	$> 3 \times 10^{19}$	$< 10^{-11}$

Infrared radiation

$$\lambda = 2.5 \text{ to } 17 \text{ }\mu\text{m}$$

$$\nu = 4000 \text{ to } 600 \text{ cm}^{-1}$$

These frequencies match the frequencies of covalent bond stretching and bending vibrations. Infrared spectroscopy can be used to find out about **covalent bonds** in molecules.

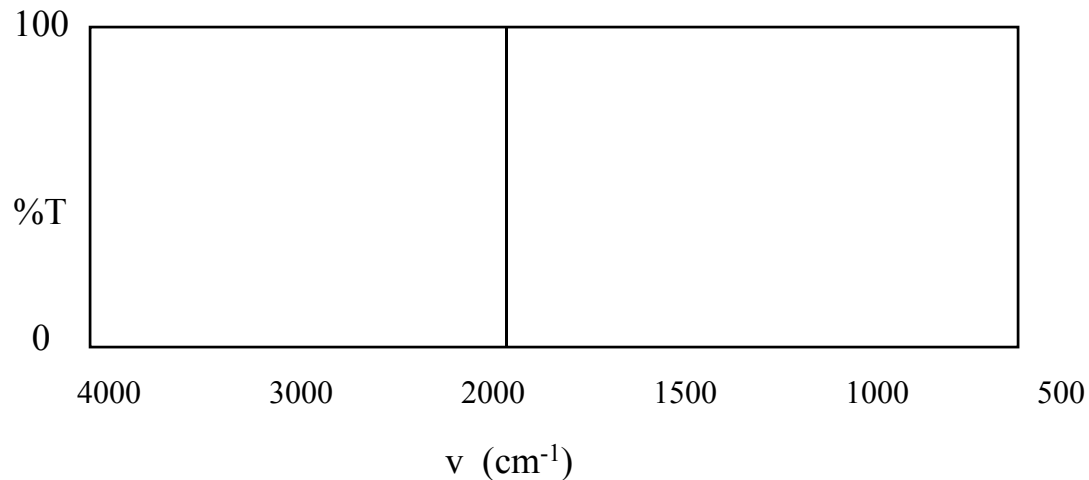
IR is used to tell:

- 1. what type of bonds are present**
- 2. some structural information**

IR source → sample → prism → detector

graph of % transmission vs. frequency

⇒ IR spectrum



HIT-NO=857

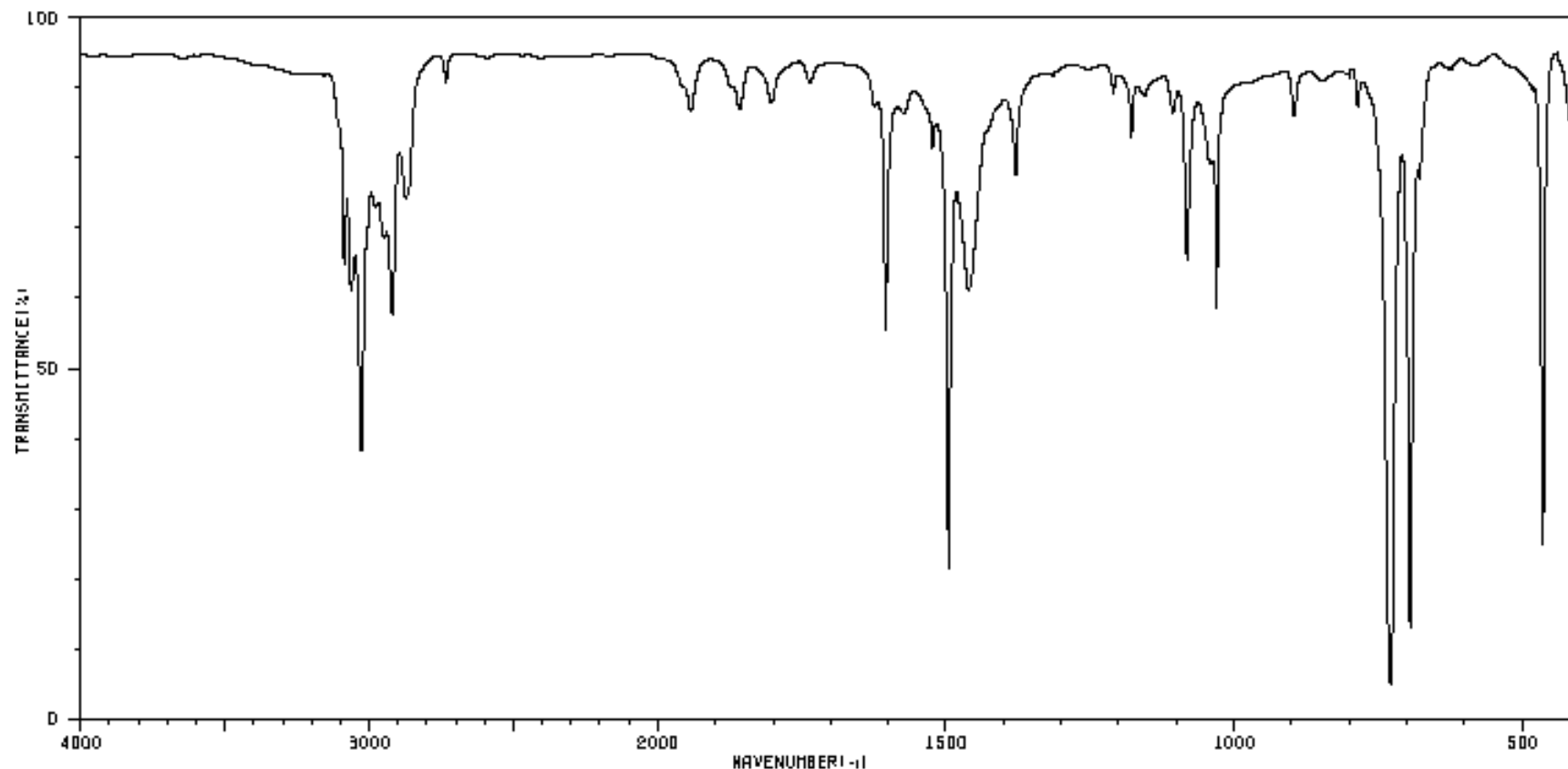
SCORE= ()

SDBS-NO=97

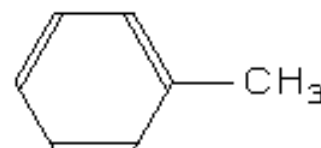
IR-NIDA-63542 : LIQUID FILM

TOLUENE

toluene

 C_7H_8 

3087	62	1868	84	1210	86	896	81
3062	58	1803	84	1179	79	786	84
3026	37	1605	55	1156	86	729	4
2948	66	1624	78	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		



Some characteristic infrared absorption frequencies

<u>BOND</u>	<u>COMPOUND TYPE</u>	<u>FREQUENCY RANGE, cm⁻¹</u>
C-H	alkanes	2850-2960 and 1350-1470
	alkenes	3020-3080 (m) and
	RCH=CH ₂	910-920 and 990-1000
	R ₂ C=CH ₂	880-900
	<i>cis</i> -RCH=CHR	675-730 (v)
	<i>trans</i> -RCH=CHR	965-975
	aromatic rings	3000-3100 (m) and
	monosubst.	690-710 and 730-770
	<i>ortho</i> -disubst.	735-770
	<i>meta</i> -disubst.	690-710 and 750-810 (m)
	<i>para</i> -disubst.	810-840 (m)
	alkynes	3300
O-H	alcohols or phenols	3200-3640 (b)
C=C	alkenes	1640-1680 (v)
	aromatic rings	1500 and 1600 (v)
C≡C	alkynes	2100-2260 (v)
C-O	primary alcohols	1050 (b)
	secondary alcohols	1100 (b)
	tertiary alcohols	1150 (b)
	phenols	1230 (b)
	alkyl ethers	1060-1150
	aryl ethers	1200-1275(b) and 1020-1075 (m)

all abs. strong unless marked: m, moderate; v, variable; b, broad

IR spectra of **ALKANES**

C—H bond “saturated”

(sp³) **2850-2960 cm⁻¹**

+ 1350-1470 cm⁻¹

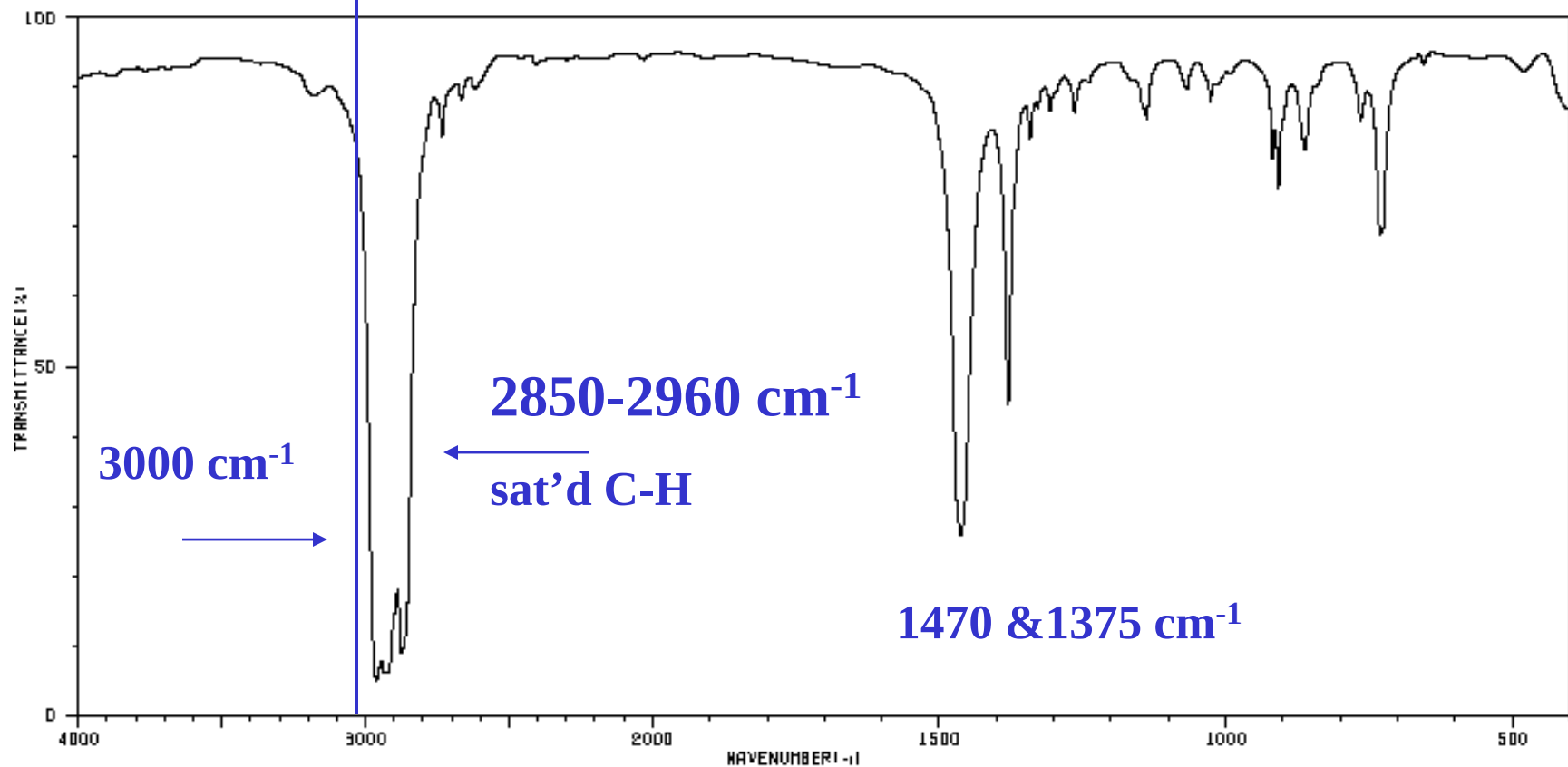
-CH₂- + 1430-1470

-CH₃ + “ and 1375

-CH(CH₃)₂ + “ and 1370, 1385

-C(CH₃)₃ + “ and 1370(s), 1395 (m)

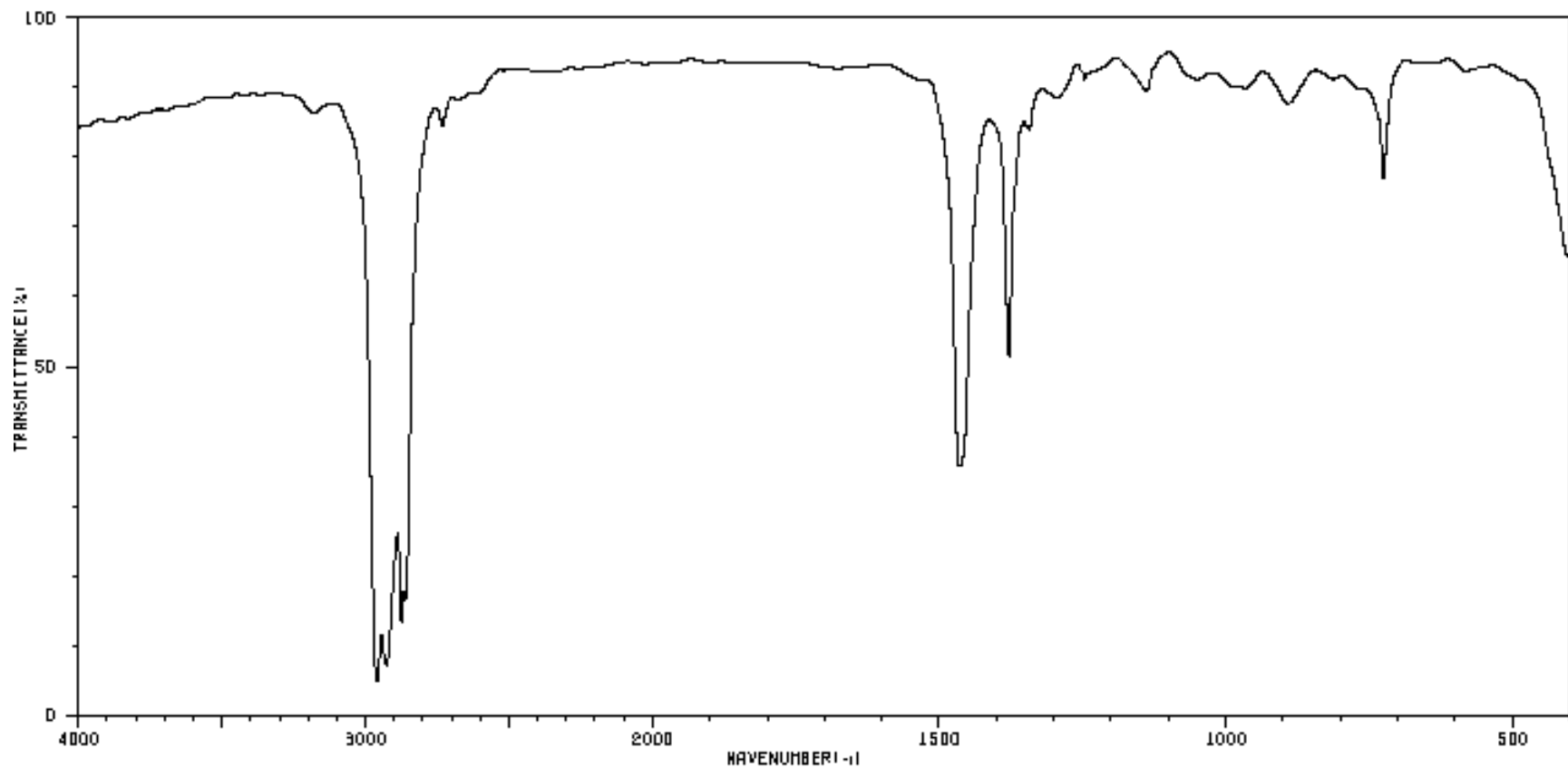
HIT-NO=1929	SCORE= ()	SDBS-NO=2475	IR-NIDA-68185 : LIQUID FILM
PENTANE			
<i>n</i> -pentane			
C ₅ H ₁₂			



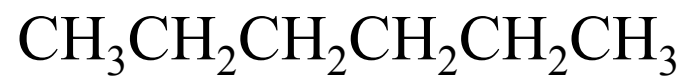
3182	86	2619	86	1138	81	732	66
3172	86	1462	24	1068	86		
2961	4	1380	45	1027	84		
2928	6	1342	79	919	77		
2875	8	1307	84	908	72		
2733	79	1264	84	862	79		
2666	84	1144	84	766	81		



HIT-NO=1737	SCORE= ()	SDBS-NO=2118	IR-NIDA-14110 : LIQUID FILM
HEXANE			
<i>n</i> -hexane			
C_6H_{14}			



3187	84	1466	34	726	74
3176	84	1379	49		
2959	4	1300	84		
2928	7	1294	84		
2875	13	1138	86		
2862	15	891	84		
2734	81	884	84		

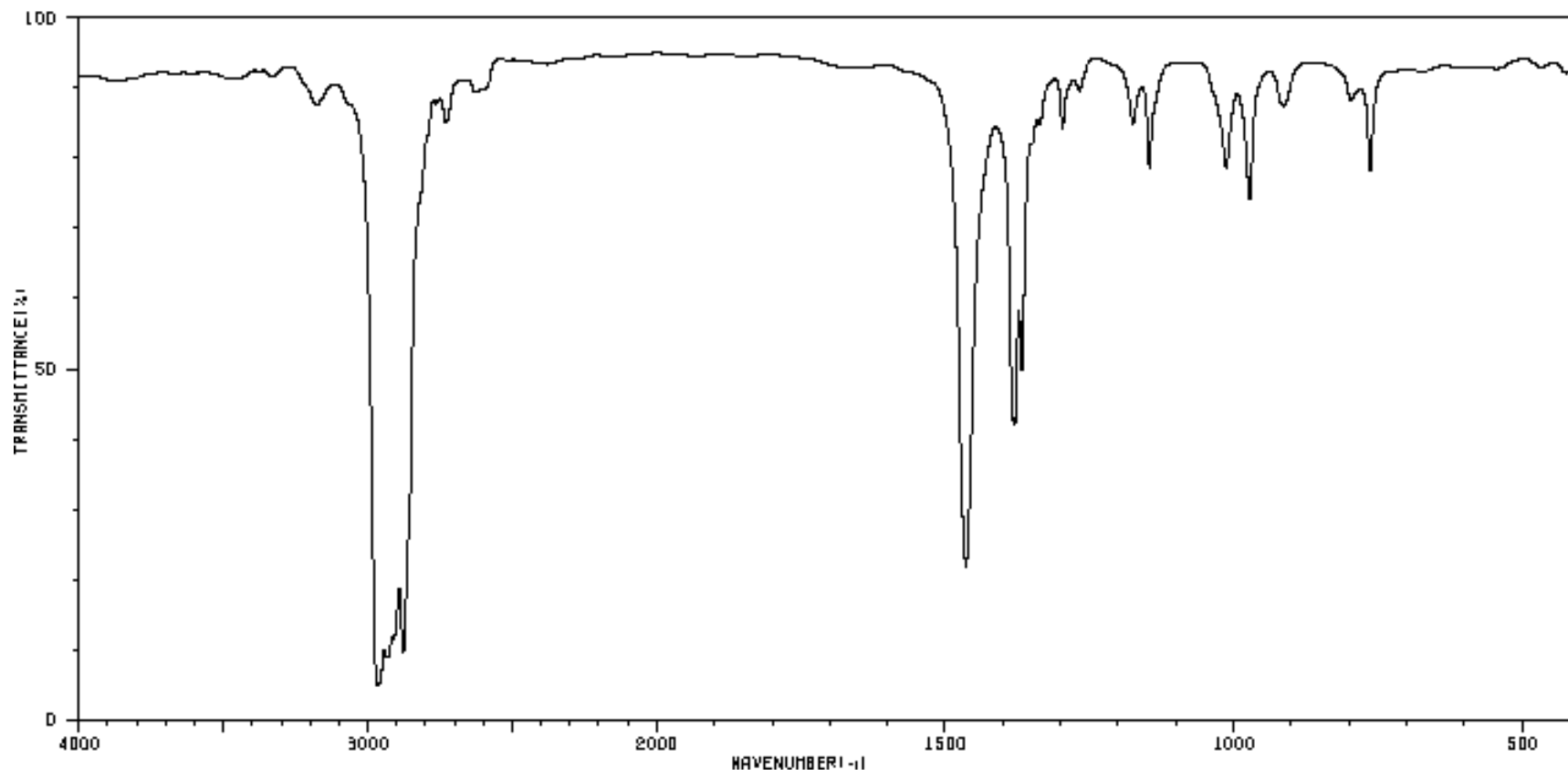


HIT-NO=4225 SCORE= () SDBS-NO=10633 IR-NIDA-03327 : LIQUID FILM

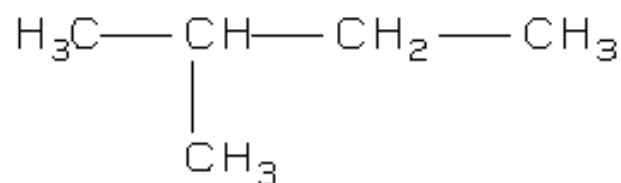
ISOPENTANE

2-methylbutane (isopentane)

C_5H_{12}



3176	84	1464	21	1013	77
2964	4	1380	41	972	70
2933	6	1368	47	913	84
2878	9	1297	81	797	84
2733	81	1268	86	764	74
2627	86	1175	81		
2604	86	1147	77		

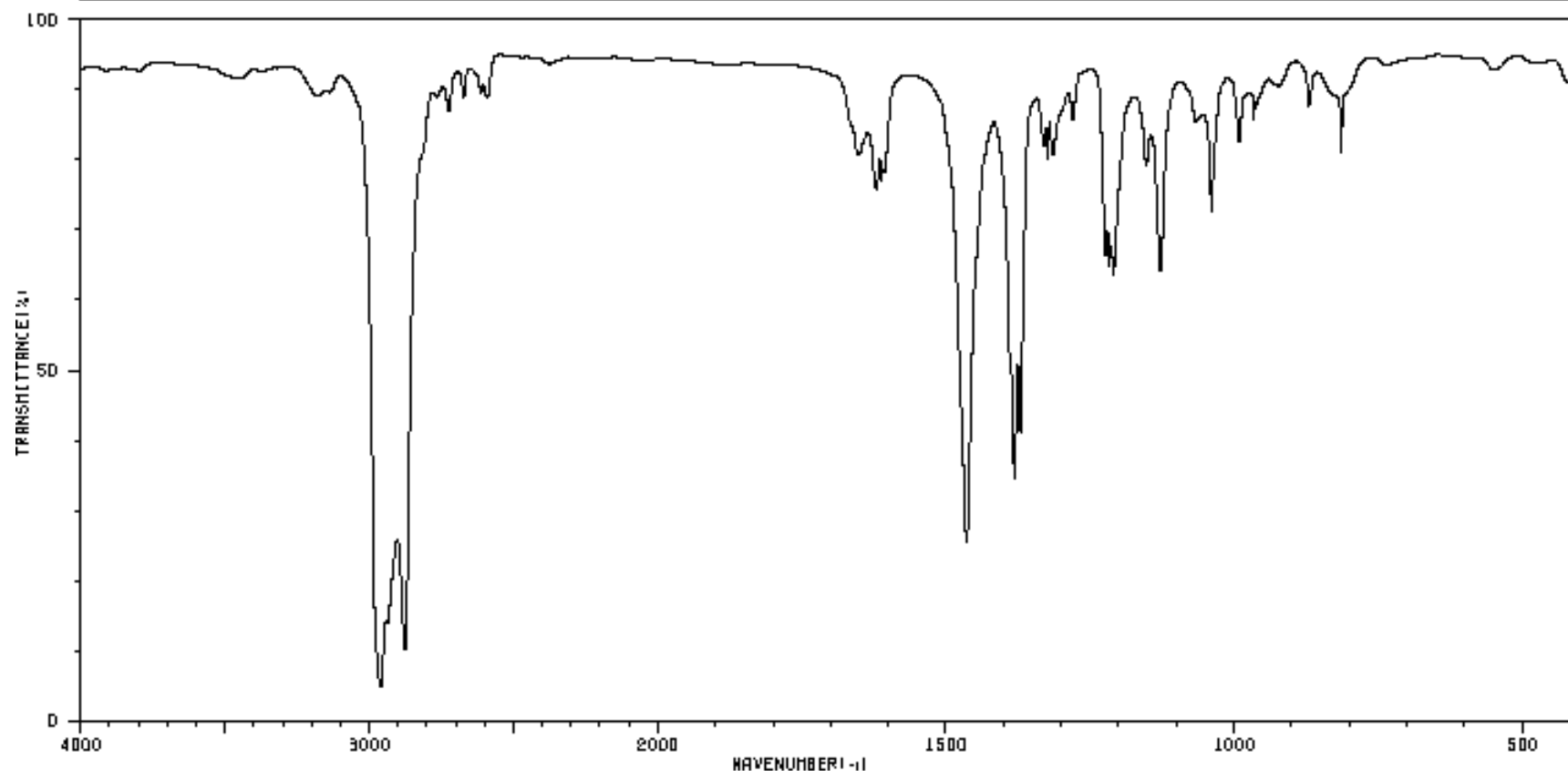


HIT-NO=1104 SCORE= () SDBS-NO=654 IR-NIDA-02888 : LIQUID FILM

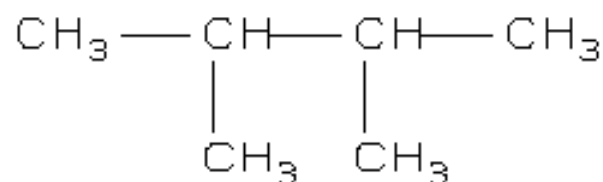
2,3-DIMETHYLBUTANE

2,3-dimethylbutane

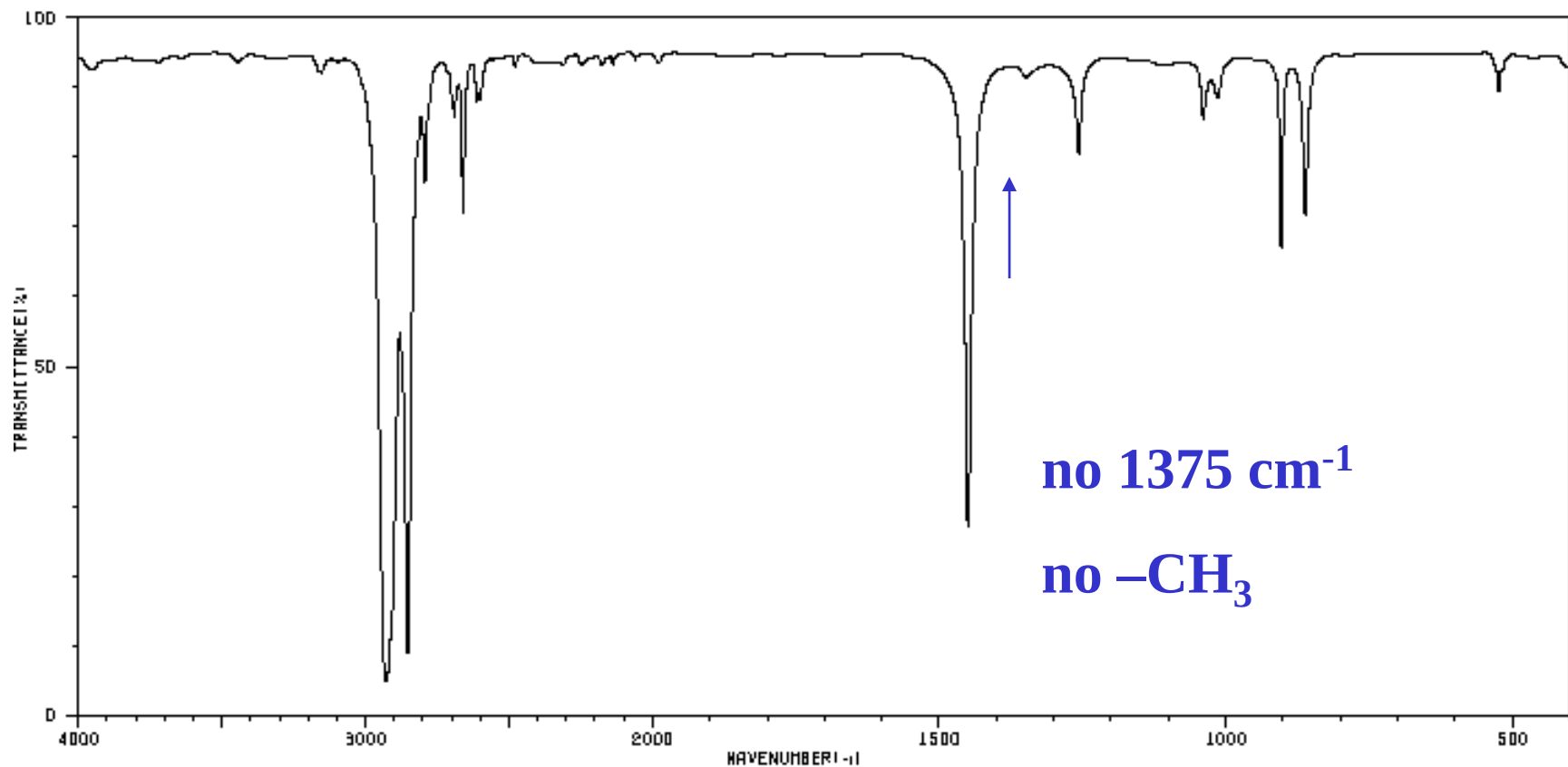
C_6H_{14}



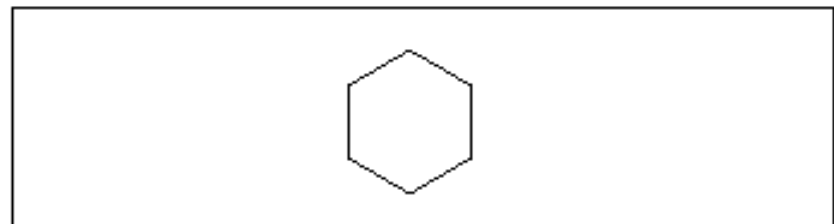
3176	86	2991	86	1381	33	1218	62	960	84
2959	4	1651	77	1371	39	1209	60	870	84
2938	13	1621	72	1330	79	1153	77	823	66
2876	9	1613	74	1323	77	1128	62	814	79
2722	84	1607	74	1315	77	1039	70		
2673	86	1454	24	1280	81	991	79		
2614	86	1389	48	1223	64	966	81		



HIT-NO=1236	SCORE= ()	SDBS-NO=897	IR-NIDA-05221 : LIQUID FILM
CYCLOHEXANE			
cyclohexane			
C_6H_{12}			



2928	4	1460	26
2853	8	1257	77
2794	72	1039	81
2690	81	1016	84
2661	70	904	64
2613	84	862	68
2599	84	624	86



IR of **ALKENES**

=C—H bond, “unsaturated” vinyl

(sp²) **3020-3080 cm⁻¹**

+ 675-1000

RCH=CH₂ + 910-920 & 990-1000
$$\text{R}_2\text{C}=\text{CH}_2 \quad + \quad 880\text{-}900$$
$$cis\text{-}RCH=CHR \quad + \quad 675\text{-}730 \text{ (v)}$$
$$trans\text{-RCH=CHR} + 965\text{-}975$$

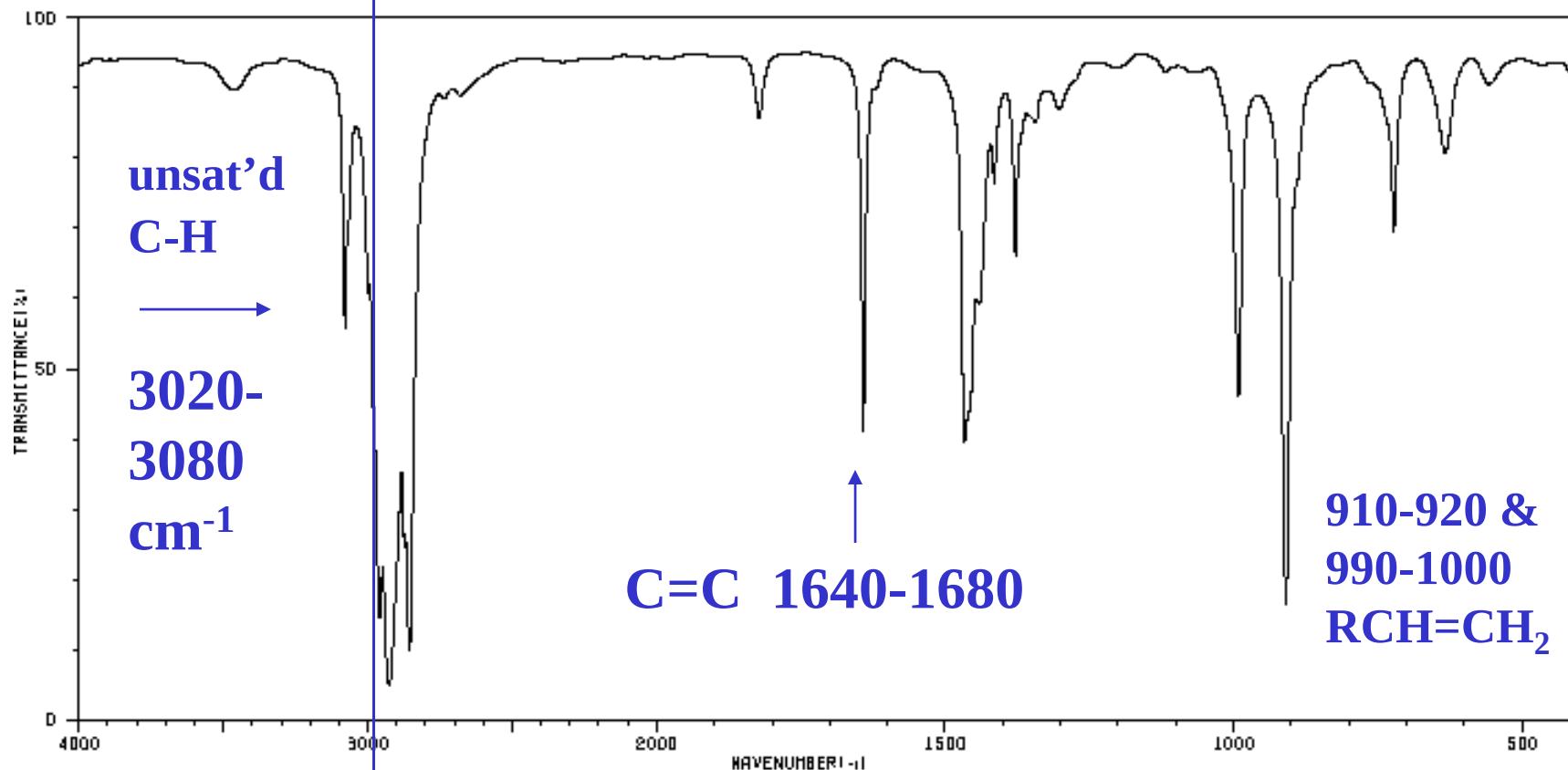
C=C bond 1640-1680 cm⁻¹ (v)

HIT-NO=1698 SCORE= () SDBS-NO=2024 IR-NIDA-04854 : LIQUID FILM

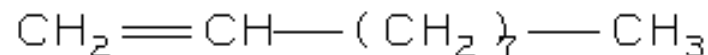
1-DECENE

1-decene

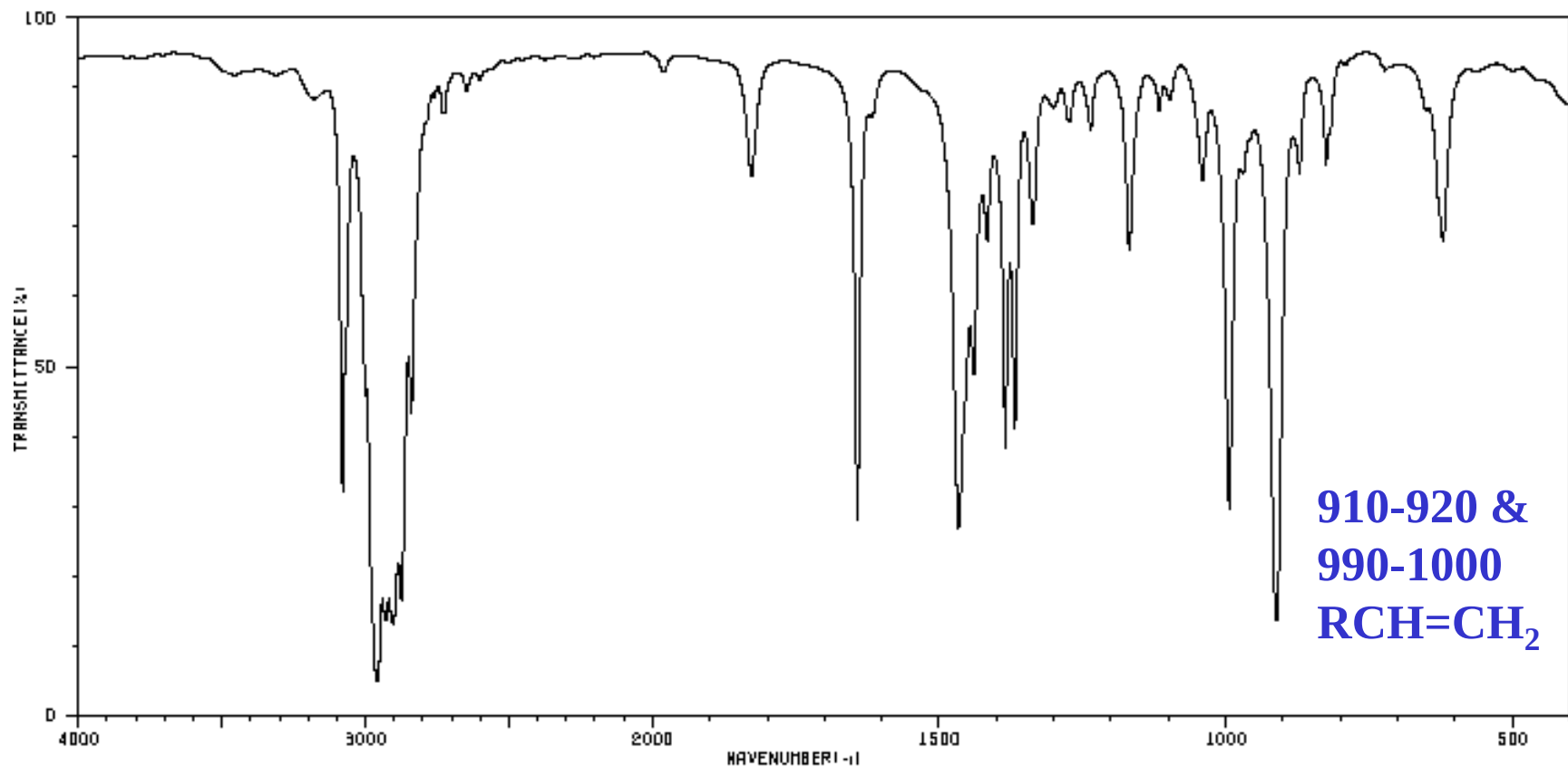
$C_{10}H_{20}$



3467	86	2874	29	1379	64
3457	86	2858	9	1343	81
3079	53	2678	86	1303	84
3068	68	1822	81	991	44
2998	58	1642	39	910	15
2958	13	1467	38	723	86
2926	4	1416	72	633	77



HIT-NO=897	SCORE= ()	SDBS-NO=212	IR-NIDA-03077 : LIQUID FILM
4-METHYL-1-PENTENE			
4-methyl-1-pentene			
C_6H_{12}			



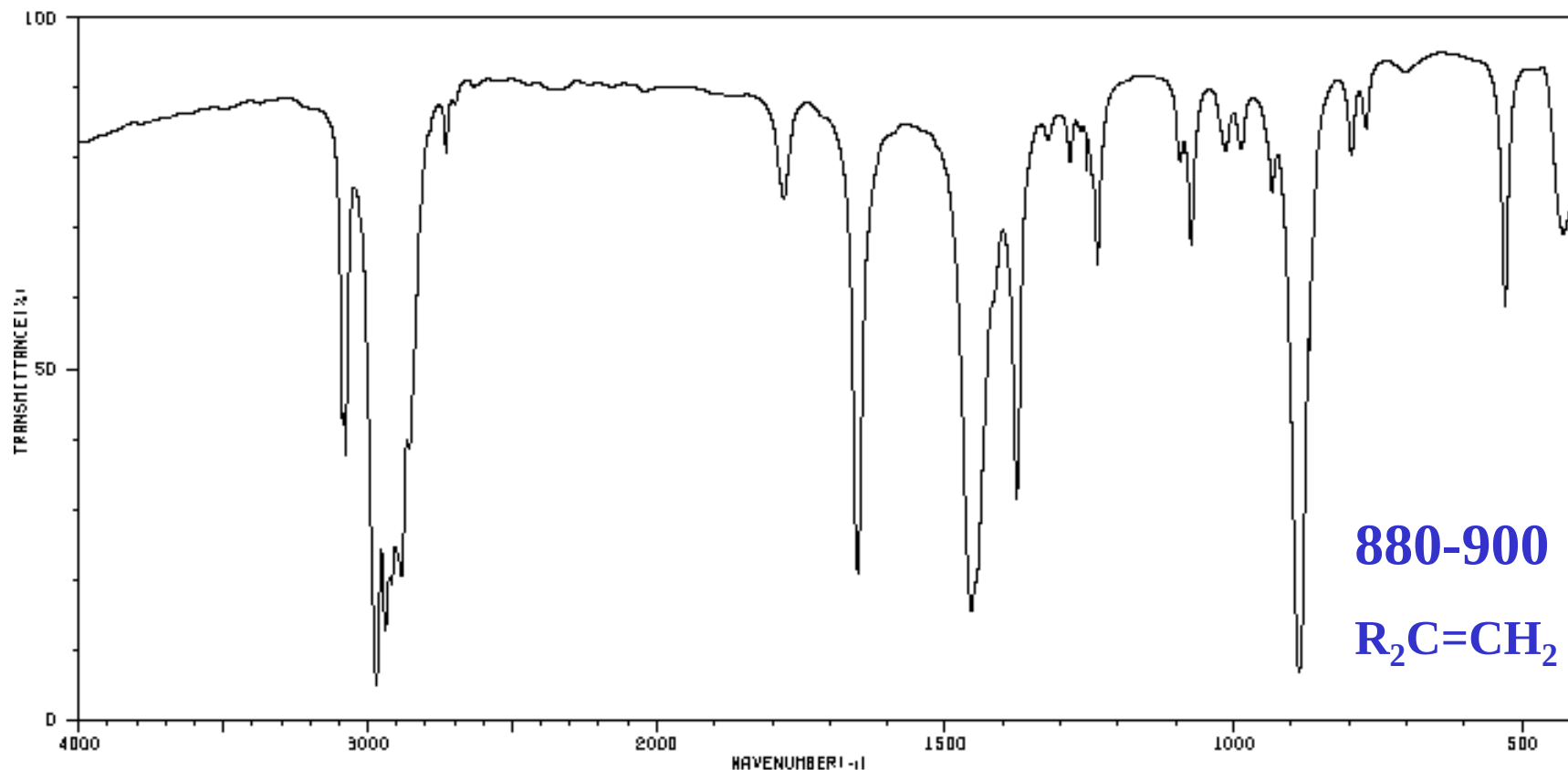
3178 84	2727 84	1386 37	1116 84	622 66	$H_2C=CH-CH_2-\underset{\begin{array}{c} \\ CH_3 \end{array}}{CH}-CH_3$
3079 31	2648 86	1368 39	1098 84		
2960 4	1828 74	1337 86	1041 74		
2929 13	1643 26	1300 84	994 28		
2904 12	1467 26	1274 81	911 13		
2874 15	1440 47	1236 81	871 74		
2839 42	1417 66	1169 64	826 77		

HIT-NO=1774 SCORE= () SDBS-NO=2176 IR-NIDA-03075 : LIQUID FILM

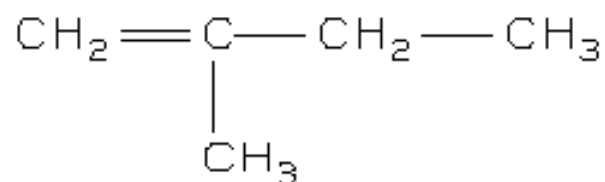
2-METHYL-1-BUTENE

2-methyl-1-butene

C₅H₁₀



3087	41	2728	77	1266	74	887	6
3077	36	1780	72	1237	62	869	50
2970	4	1651	20	1093	77	796	77
2939	12	1466	14	1074	64	770	81
2919	18	1377	30	1014	79	530	57
2883	20	1322	79	987	79	429	66
2856	37	1284	77	933	72		

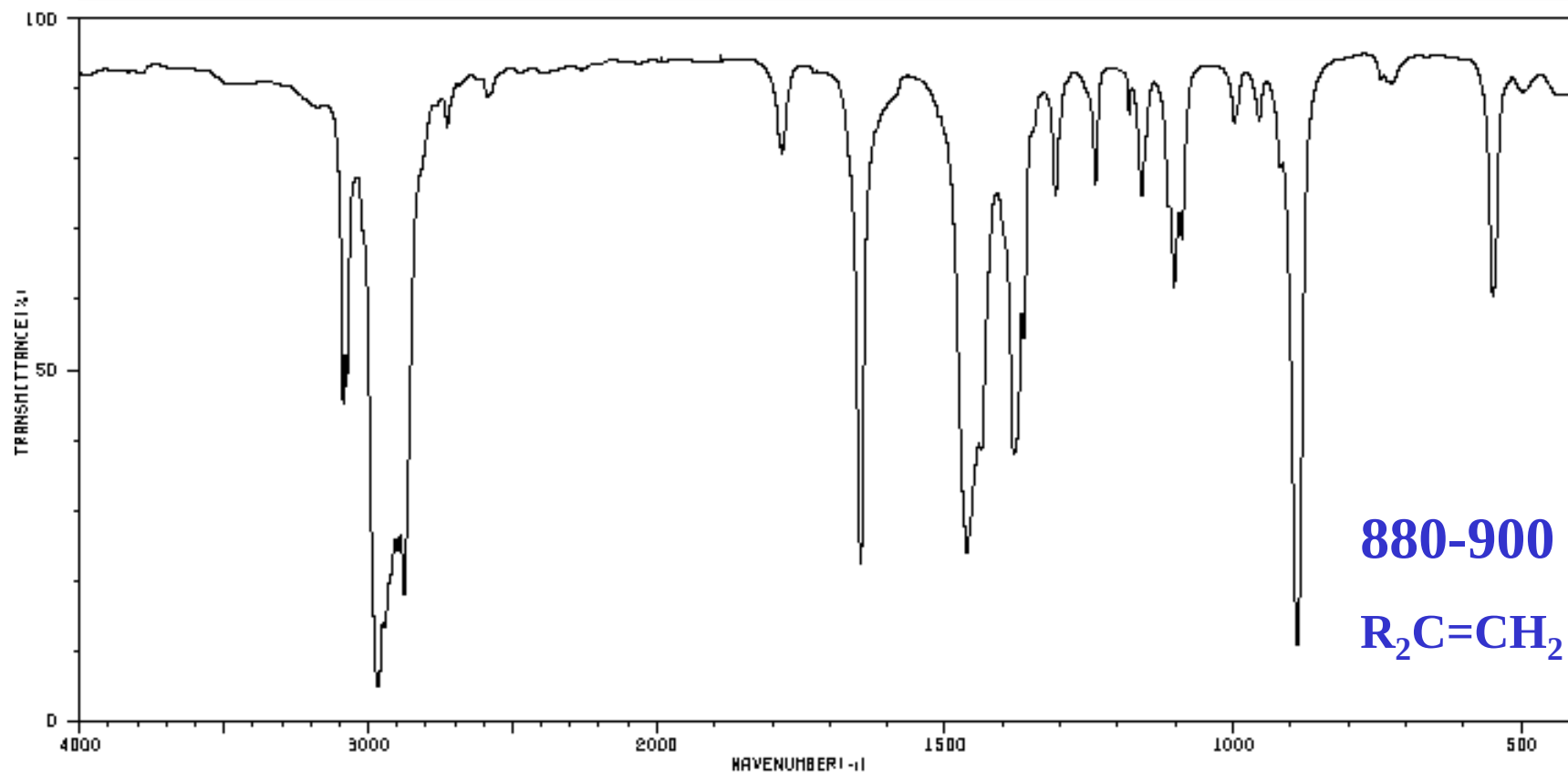


HIT-NO=2801 SCORE= () SDBS-NO=4815 IR-NIDA-03377 : LIQUID FILM

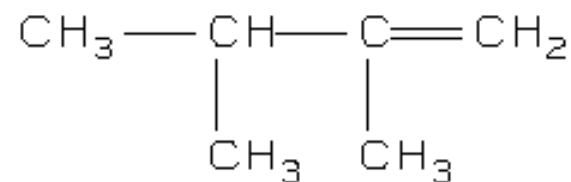
2,3-DIMETHYL-1-BUTENE

2,3-dimethyl-1-butene

C₆H₁₂



3087	43	2988	86	1308	72	966	81
3075	46	1794	84	1239	74	888	10
2966	4	1783	77	1181	84	550	58
2944	13	1646	21	1169	72	497	86
2898	23	1462	23	1102	58		
2875	17	1380	36	1089	86		
2727	81	1363	62	998	81		



IR spectra **BENZENE**s

=C—H bond, “unsaturated” “aryl”

(sp²) **3000-3100 cm⁻¹**

+ 690-840

mono-substituted + 690-710, 730-770

ortho-disubstituted + 735-770

meta-disubstituted + 690-710, 750-810(m)

para-disubstituted + 810-840(m)

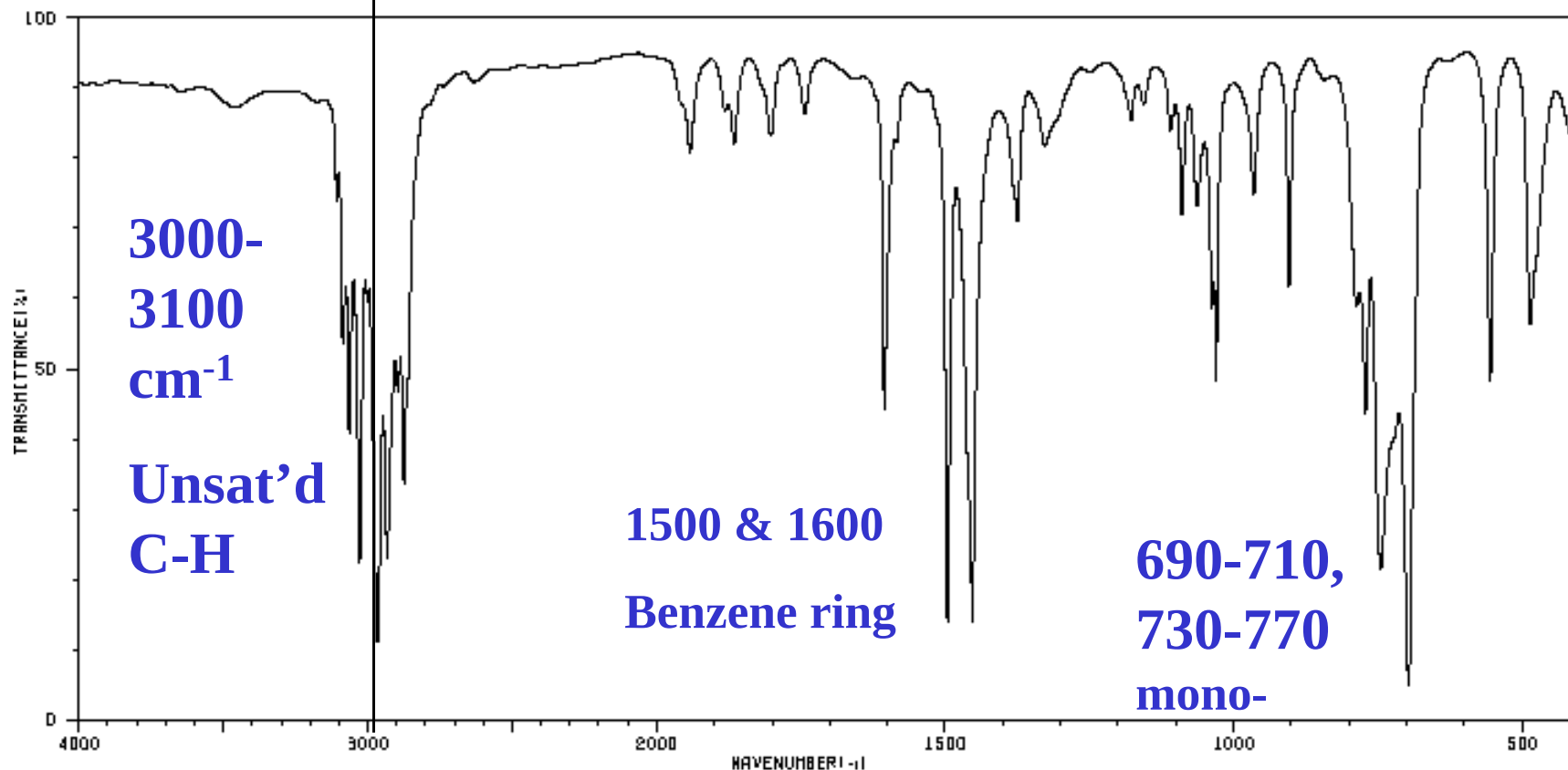
C=C bond **1500, 1600 cm⁻¹**

HIT-NO=1402 SCORE= () SDBS-NO=1332 IR-NIDA-05258 : LIQUID FILM

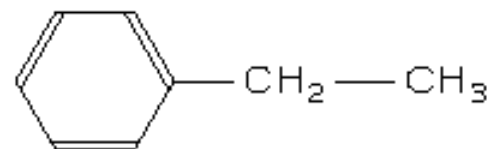
ETHYLBENZENE

ethylbenzene

C_8H_{10}



3468	84	2933	21	1802	79	1178	81	904	58
3108	70	2896	44	1744	84	1110	81	788	57
3087	52	2875	32	1606	42	1090	70	772	42
3066	39	1966	84	1496	13	1064	70	746	20
3028	21	1942	77	1453	13	1037	57	697	4
3003	57	1881	84	1376	88	1030	46	556	46
2967	10	1866	78	1329	79	966	72	486	53

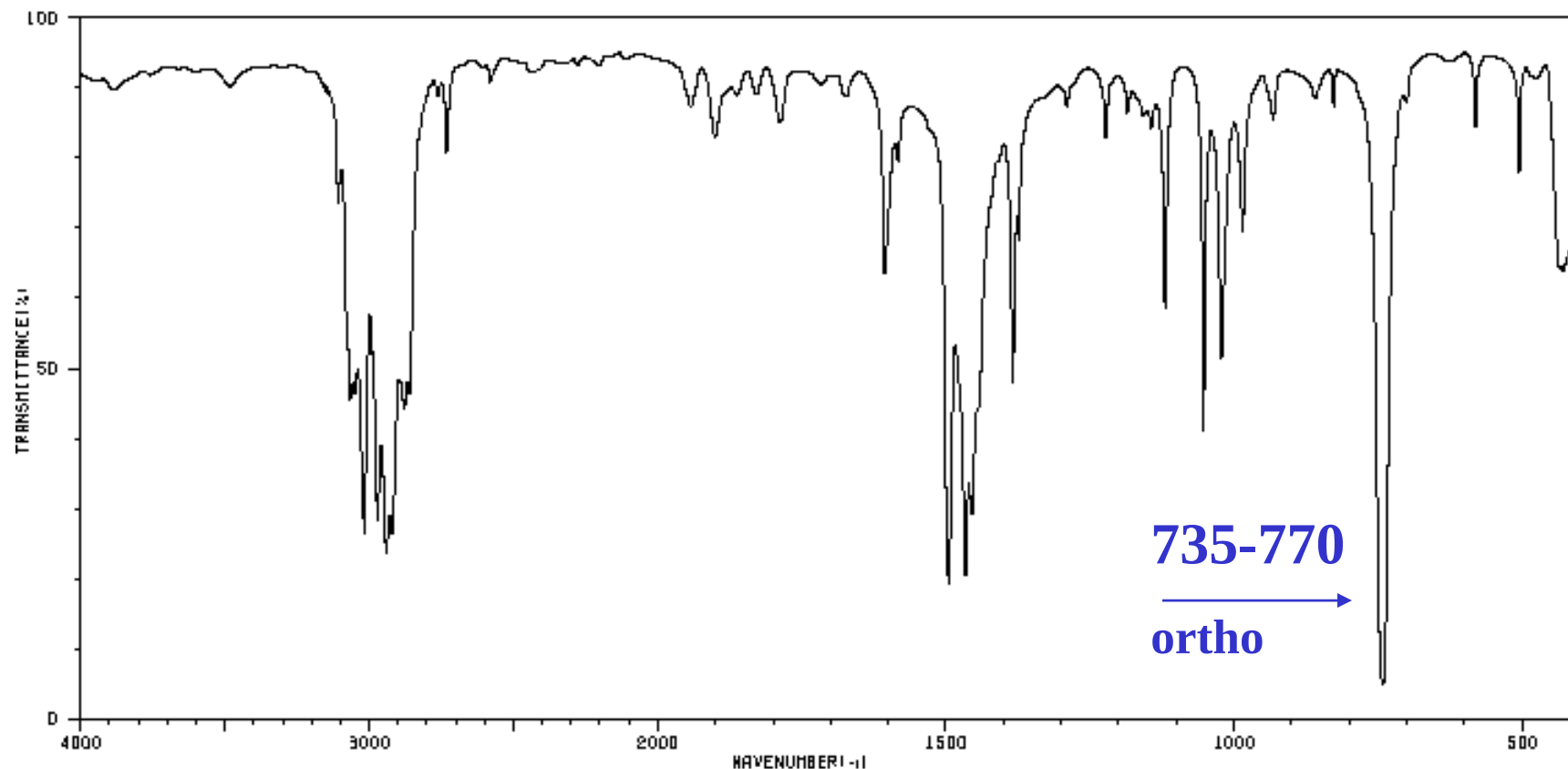


HIT-NO=1272 SCORE= () SDBS-NO=1028 IR-NIDA-21942 : LIQUID FILM

O-XYLENE

***o*-xylene**

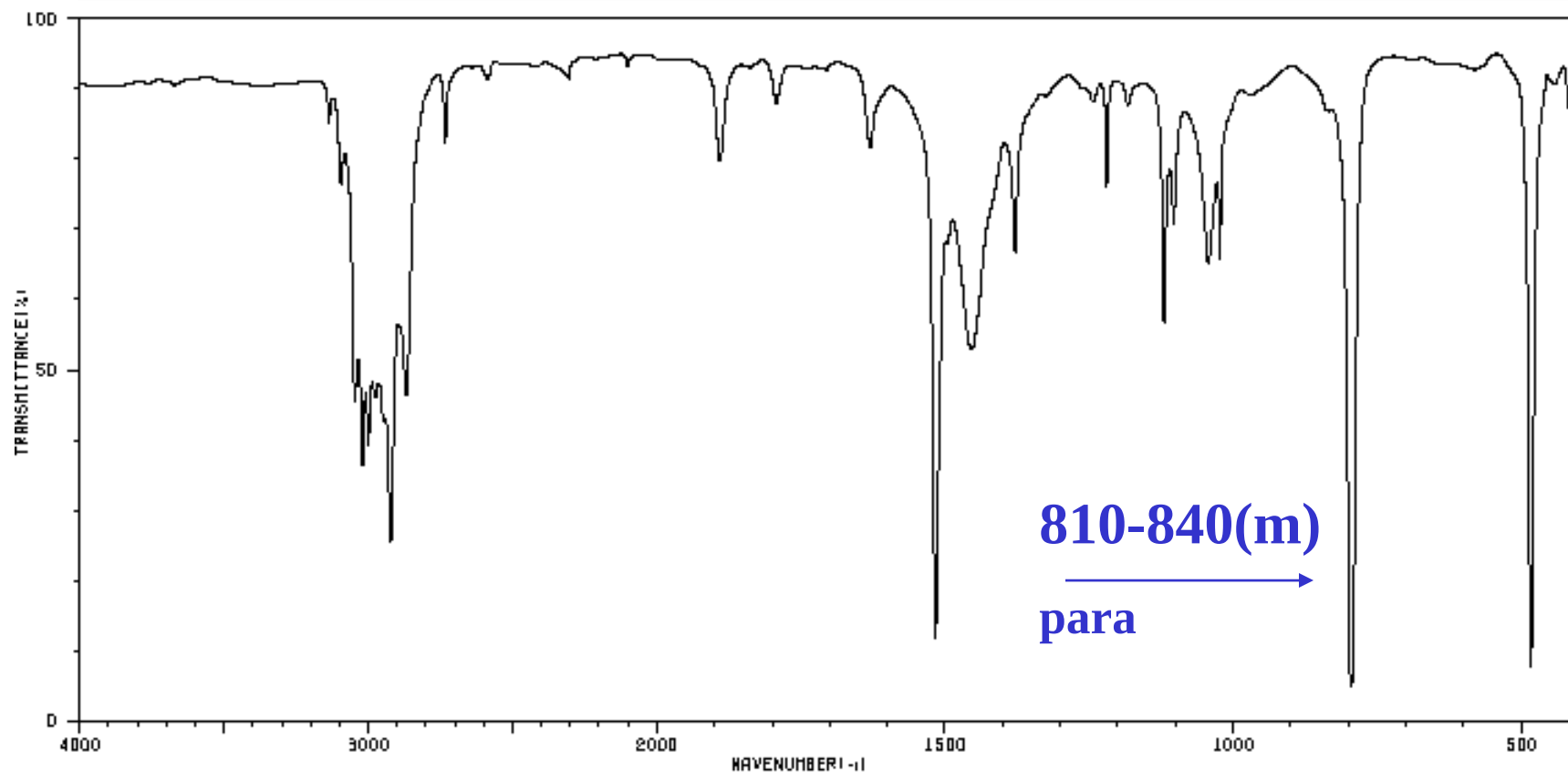
C_8H_{10}



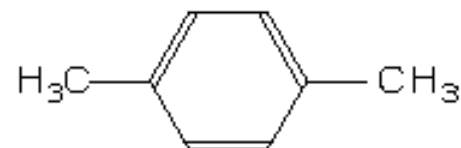
3108	70	2878	42	1683	77	1223	79	986	66
3066	43	2860	44	1495	18	1186	84	932	81
3050	44	2732	77	1467	20	1157	81	742	4
3018	26	1942	84	1466	27	1146	81	682	81
2971	26	1901	79	1384	46	1120	57	506	74
2940	22	1787	81	1374	86	1053	39	436	62
2921	26	1606	60	1291	84	1022	48	431	62

Chemical structure of *o*-xylene (1,2-dimethylbenzene): Cc1ccccc1C

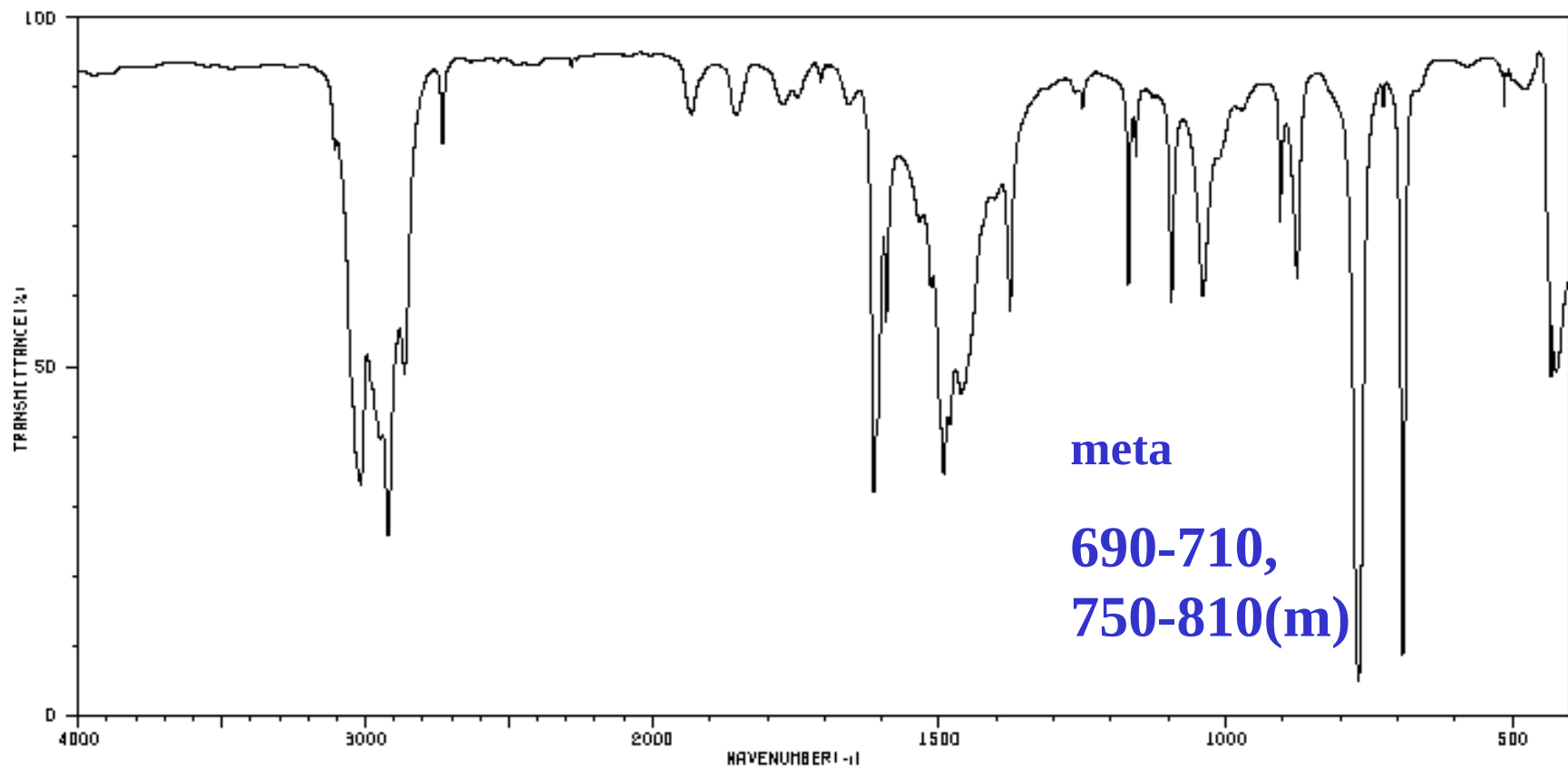
HIT-NO=1238	SCORE= ()	SDBS-NO=899	IR-NIDA-63598 : LIQUID FILM
P-XYLENE			
<i>p</i> -xylene			
C_6H_{10}			



3136	81	2923	24	1454	60	1043	62
3095	74	2868	44	1378	64	1023	64
3047	43	2733	78	1243	84	795	4
3020	36	1890	77	1220	72	484	7
3000	37	1793	84	1183	84		
2976	44	1630	78	1120	55		
2945	41	1516	11	1103	68		



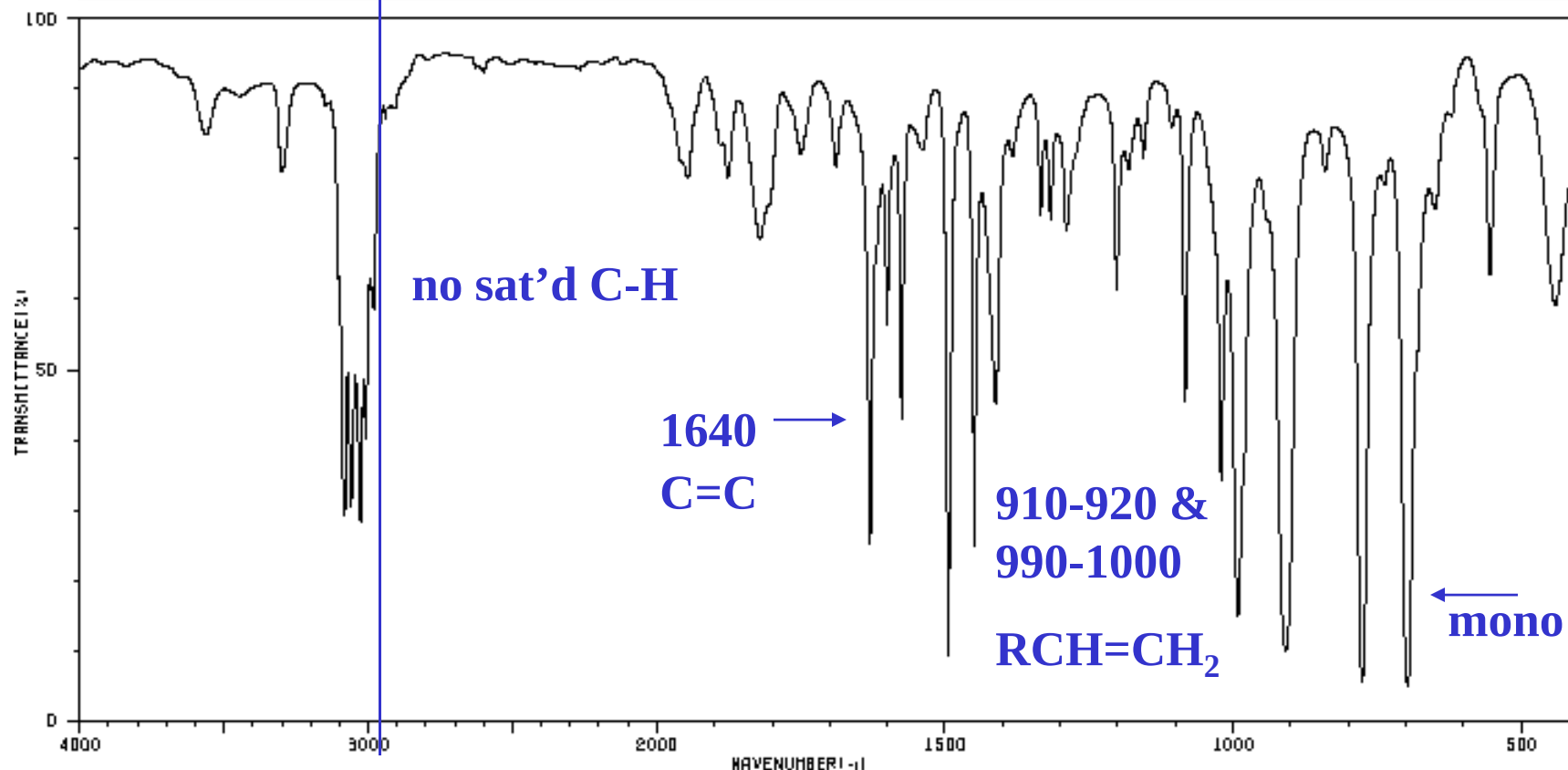
HIT-NO=1275	SCORE= ()	SDBS-NO=1032	IR-NIDA-63601 : LIQUID FILM
M-XYLENE			
<i>m</i> -xylene			
C_8H_{10}			



3106	79	1864	84	1492	33	1170	58	726	84
3016	32	1772	84	1482	39	1157	77	691	8
2948	37	1764	84	1462	44	1095	57	515	64
2921	24	1668	84	1376	55	1040	57	483	86
2864	47	1614	31	1263	86	905	68	478	86
2732	79	1592	59	1256	86	876	60	434	46
1932	84	1516	58	1250	84	769	4		

H_3C $-CH_3$

HIT-NO=2170	SCORE= ()	SDBS-NO=3044	IR-NIDA-10290 : LIQUID FILM
STYRENE			
C_6H_6			



3299	74	1946	74	1496	9	1202	68	841	74
3082	28	1876	74	1449	23	1182	74	777	5
3060	29	1821	66	1412	43	1156	77	736	72
3027	27	1688	77	1383	77	1083	43	698	4
3009	38	1630	24	1334	70	1021	33	650	70
2980	57	1601	59	1317	88	992	14	555	60
1955	77	1576	41	1290	66	909	9	442	67

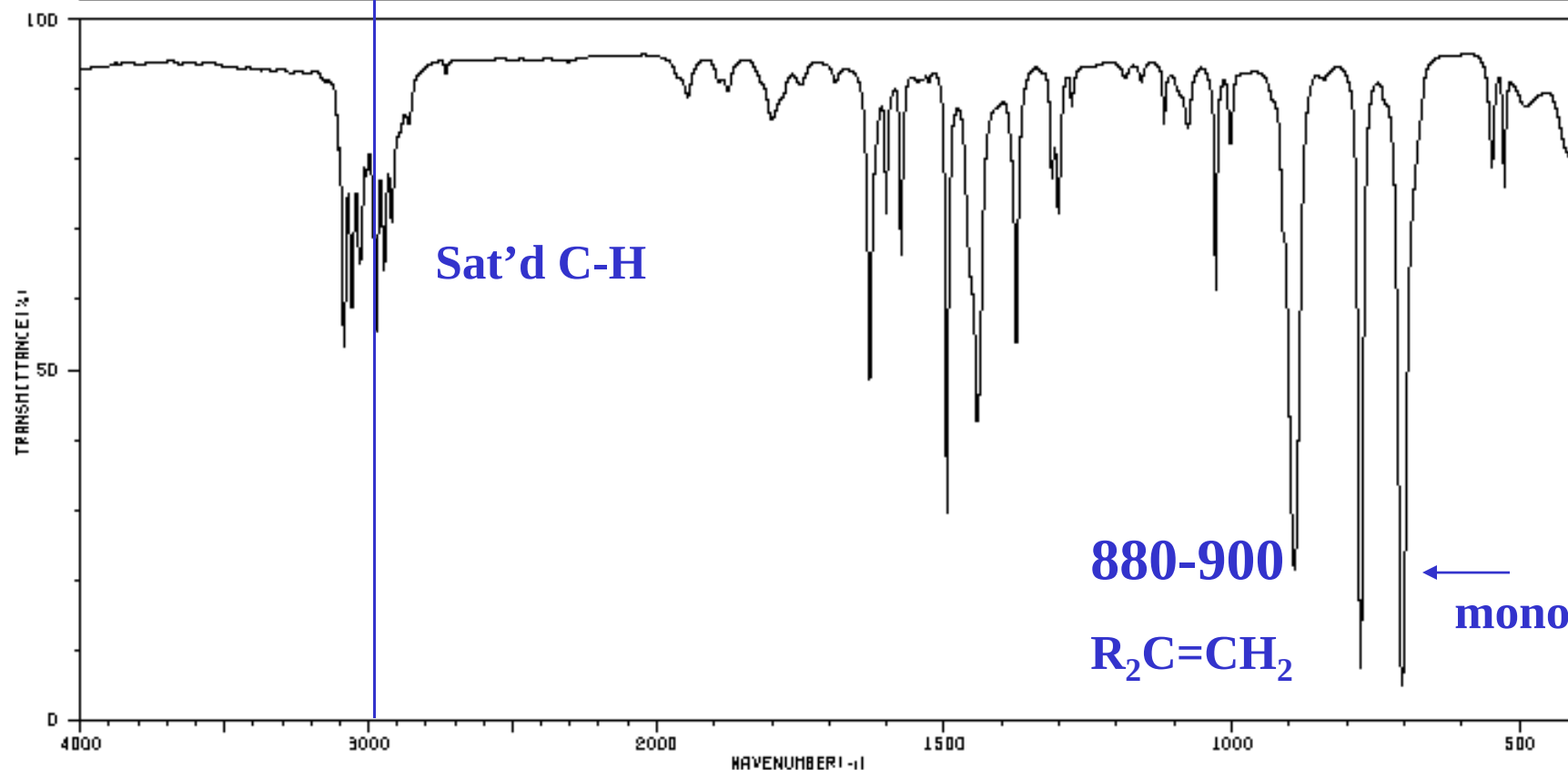
C=Cc1ccccc1

HIT-NO=1854 SCORE= () SDBS-NO=2368 IR-NIDA-00385 : LIQUID FILM

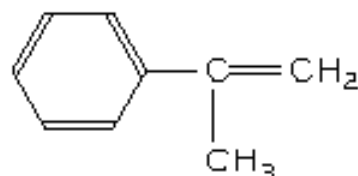
ISOPROPENYLBENZENE

2-phenylpropene

C₉H₁₀



3086	60	2951	81	1496	28	1077	81	627	72
3058	57	1946	86	1443	41	1028	58	488	84
3033	82	1878	86	1375	52	1003	79		
3008	74	1800	81	1313	74	892	20		
2974	53	1630	46	1302	70	777	7		
2946	62	1601	70	1279	84	704	4		
2920	68	1576	64	1118	81	648	77		

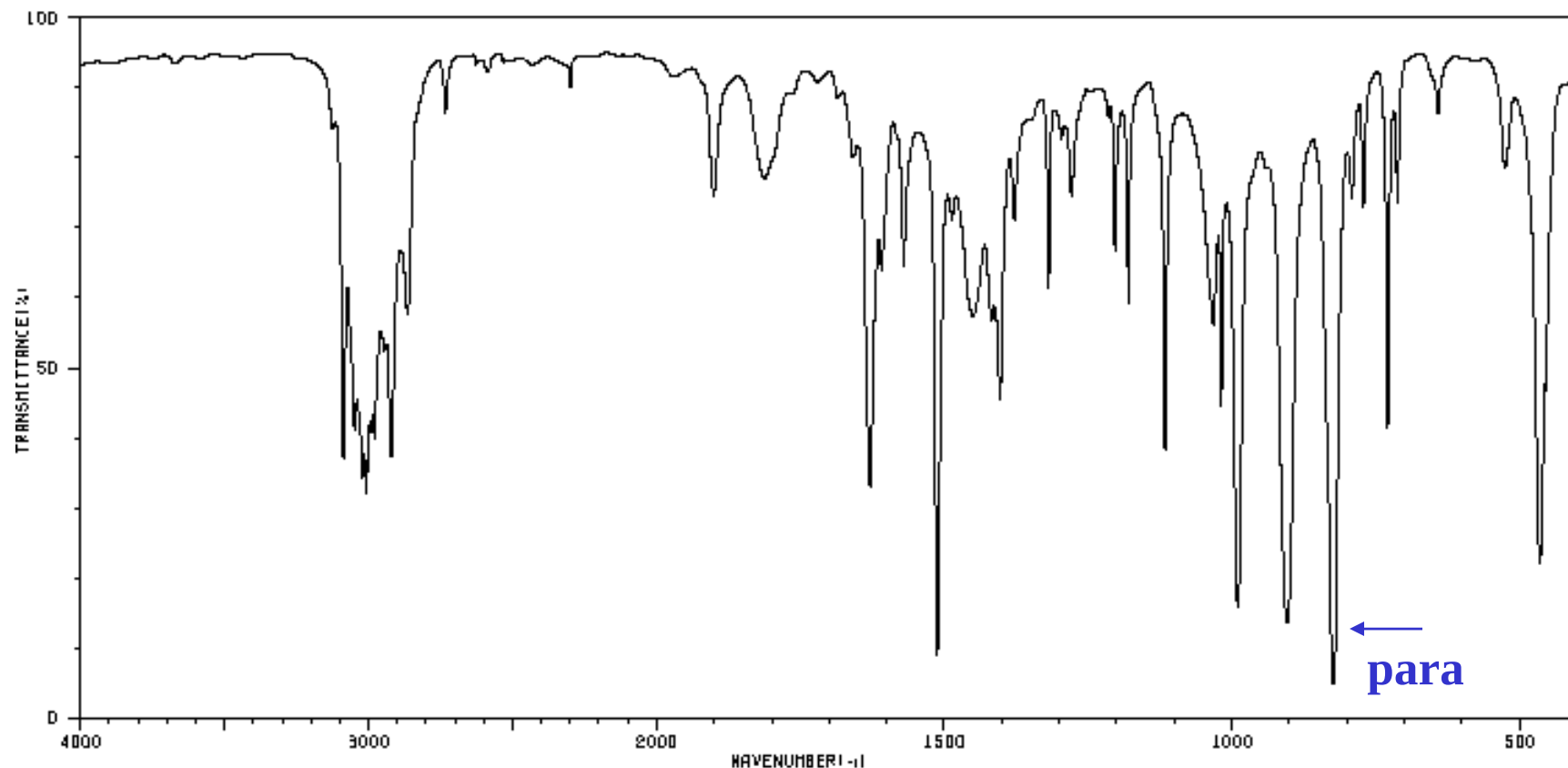


HIT-NO=3320 SCORE= () SDBS-NO=6328 IR-NIDA-09901 : LIQUID FILM

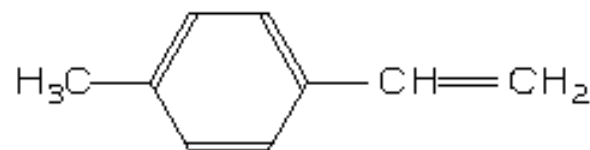
P-METHYLSTYRENE

p-methylstyrene

C₉H₁₀



3087	36	2922	36	1487	68	1204	64	824	4
3048	39	2864	55	1450	55	1181	57	792	72
3020	33	1901	72	1416	55	1116	36	772	70
3007	31	1629	32	1403	43	1032	63	730	39
2993	38	1609	60	1378	68	1018	43	712	70
2980	36	1571	62	1319	58	990	15	466	21
2946	60	1513	8	1279	72	904	19	457	43



IR spectra **ALCOHOLS & ETHERS**

C—O bond **1050-1275 (b) cm⁻¹**

1° ROH 1050

2° ROH 1100

3° ROH 1150

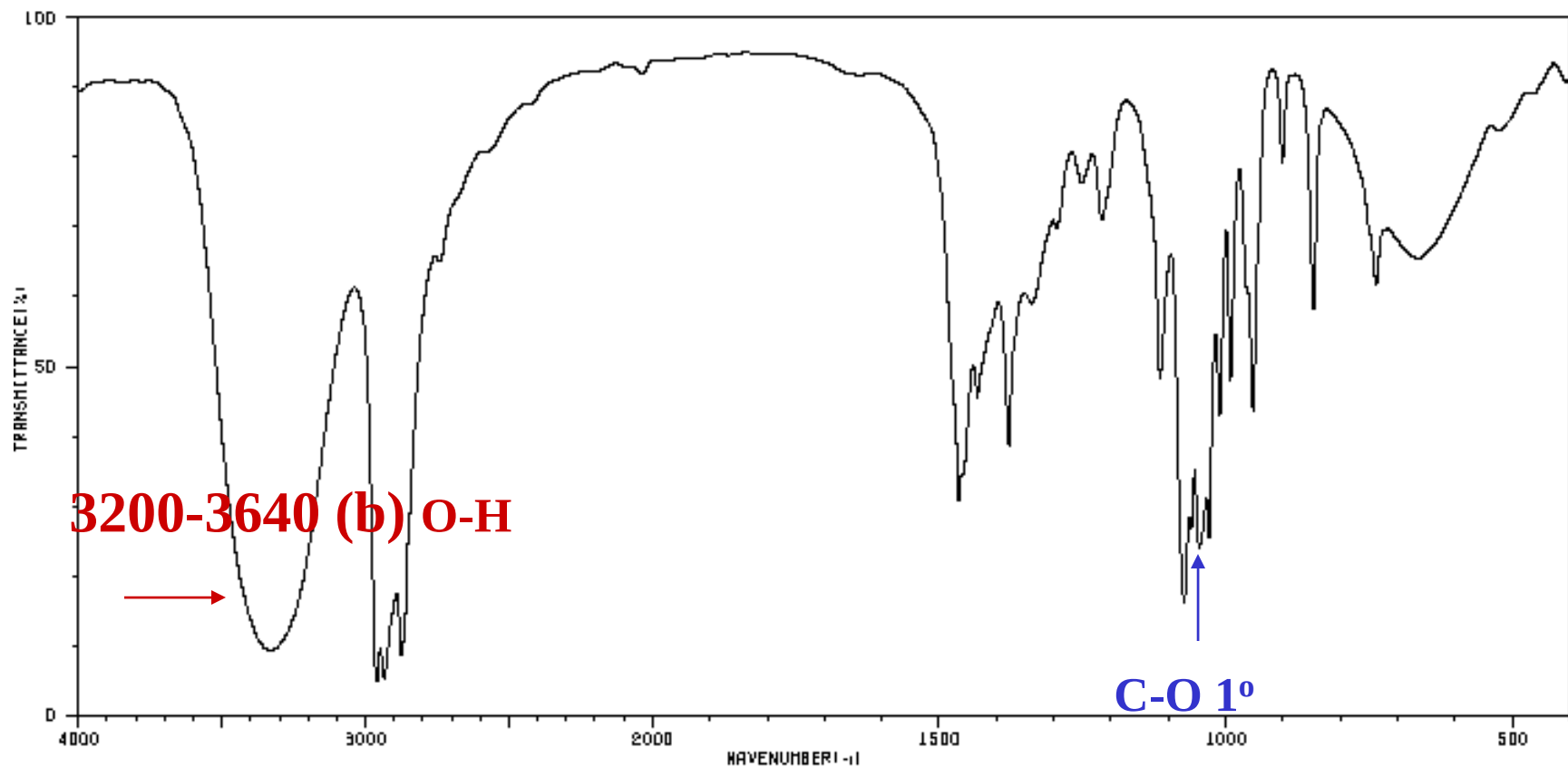
ethers 1060-1150

O—H bond **3200-3640 (b)**



HIT-NO=1418	SCORE= ()	SDBS-NO=1374	IR-NIDA-05408 : LIQUID FILM
1-BUTANOL			
$C_4H_{10}O$			

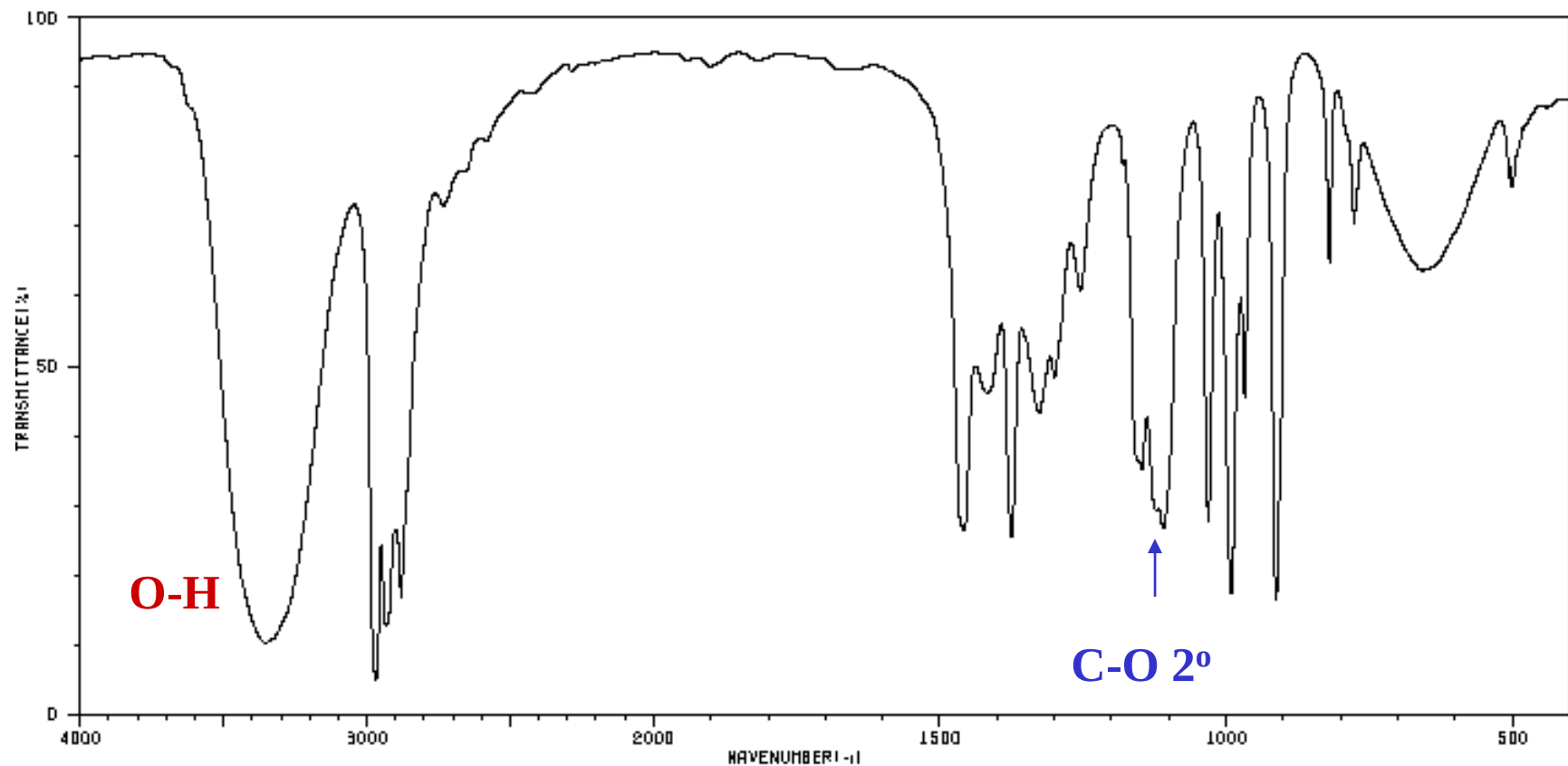
1-butanol



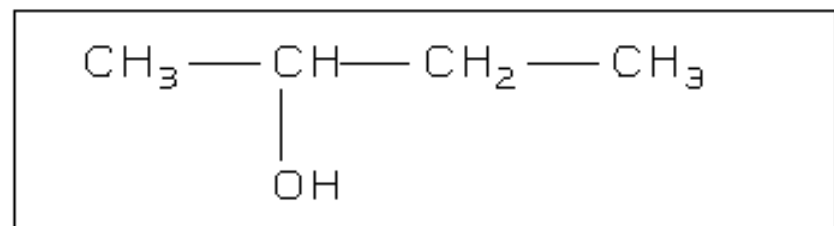
3333	9	1434	49	1073	16	901	77
3323	9	1379	37	1060	26	847	57
2960	4	1338	57	1047	23	738	58
2934	6	1296	68	1029	24	670	62
2875	8	1252	74	1011	42	665	62
1466	30	1217	68	992	46		
1461	33	1116	46	963	42		



HIT-NO=1035	SCORE= ()	SDBS-NO=507	IR-NIDA-04700 : LIQUID FILM
2-BUTANOL			
$C_4H_{10}O$			



3363	10	1376	24	1110	26	666	60
2968	4	1327	42	1031	26	651	60
2932	12	1300	46	991	16	501	72
2880	16	1266	68	968	43		
2734	70	1154	35	913	15		
1457	25	1148	34	820	82		
1416	44	1122	28	777	68		

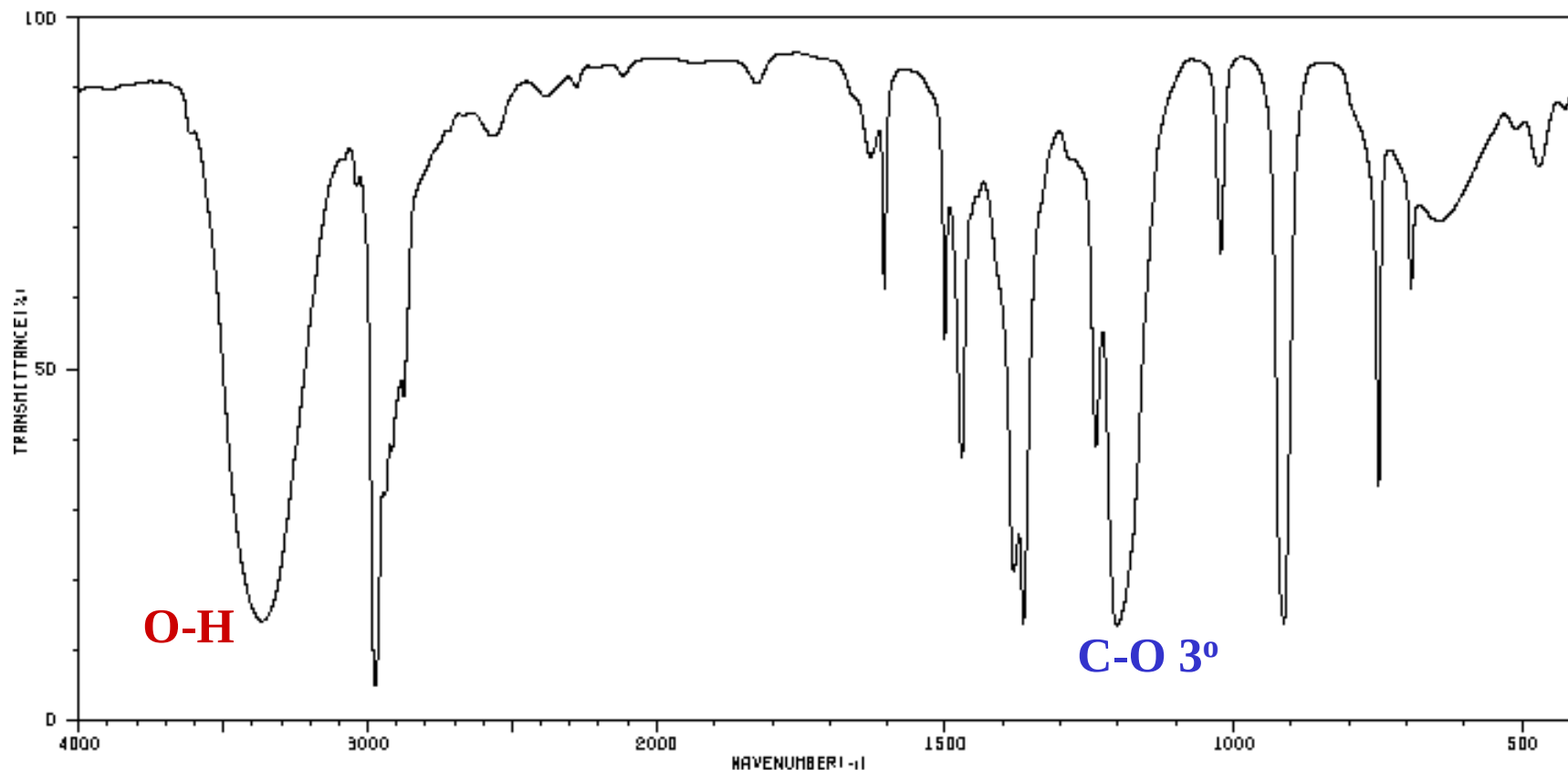


HIT-NO=1034 SCORE= () SDBS-NO=506 IR-NIDA-05409 : LIQUID FILM

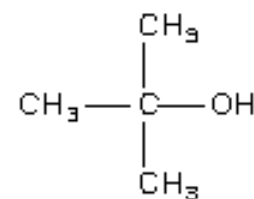
2-METHYL-2-PROPANOL

tert-butyl alcohol

C₄H₁₀O



3365	13	1630	77	1202	12	511	81
3038	72	1606	58	1022	64	471	77
2974	4	1501	52	913	13		
2940	31	1471	36	749	32		
2875	44	1381	20	693	58		
2564	79	1365	19	646	68		
2385	86	1239	37	643	68		



methyl *n*-propyl ether



C-O ether

$$\text{CH}_3 - (\text{CH}_2)_2 - \text{O} - \text{CH}_3$$

HIT-NO=1228

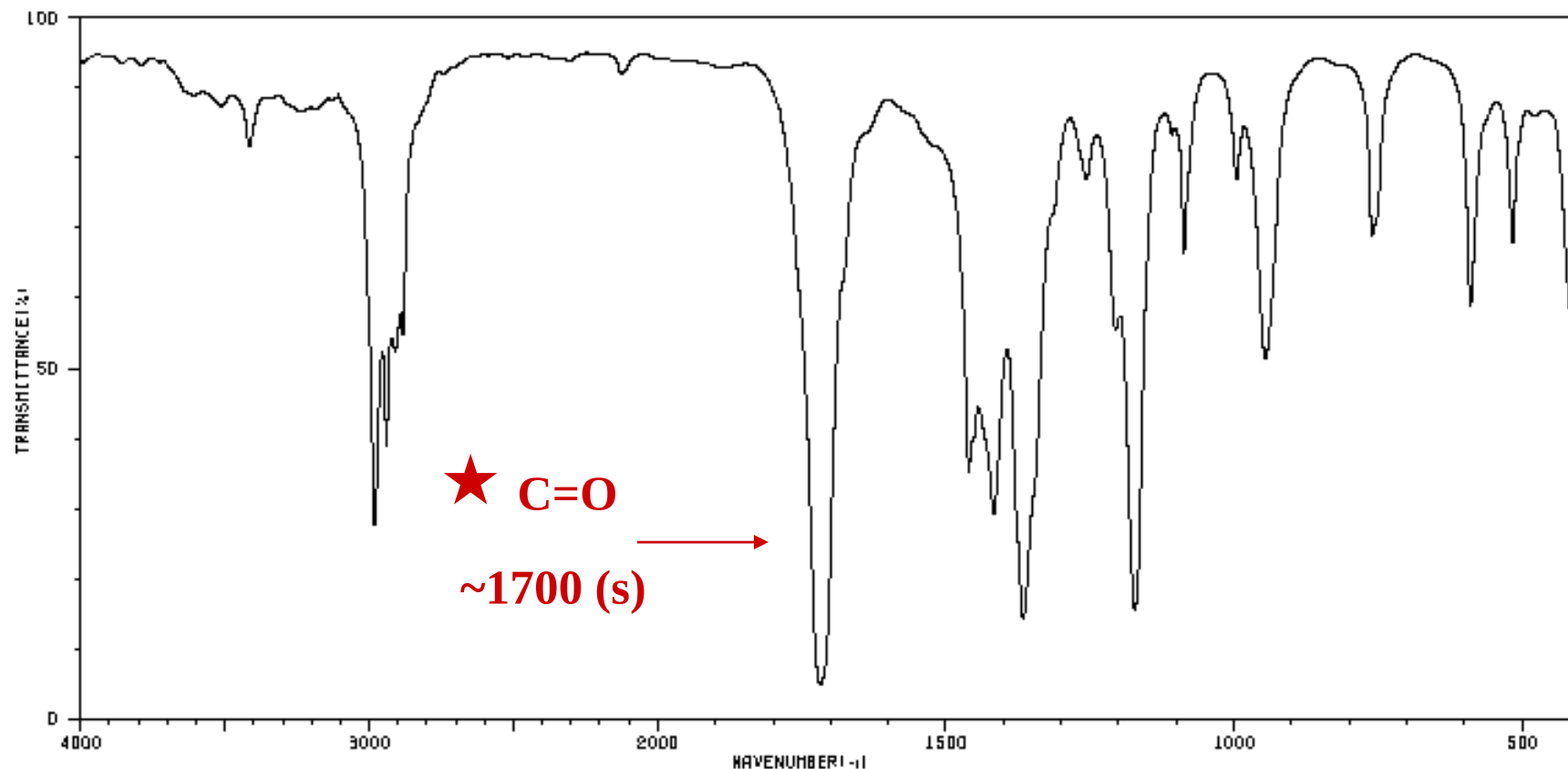
SCORE= ()

SDBS-NO=888

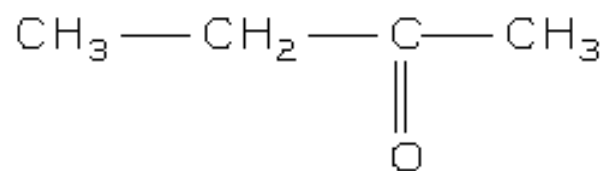
IR-NIDA-33689 : LIQUID FILM

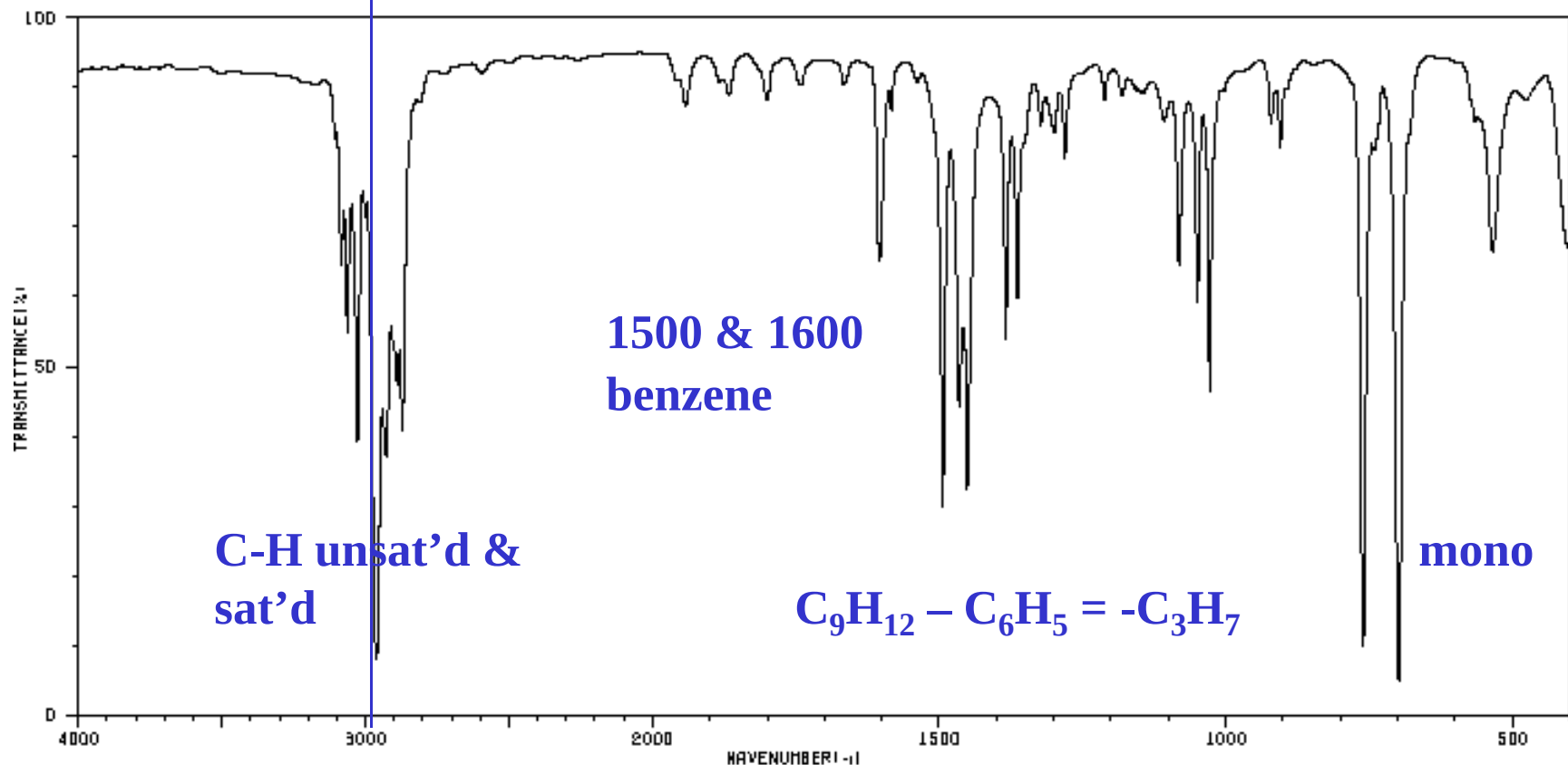
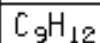
2-BUTANONE

2-butanone

 C_4H_8O 

3611	84	1718	4	1173	14
3416	79	1461	34	1087	64
2981	26	1454	38	996	74
2964	44	1417	27	946	49
2940	37	1366	13	761	66
2909	50	1257	74	590	57
2883	62	1206	69	617	66



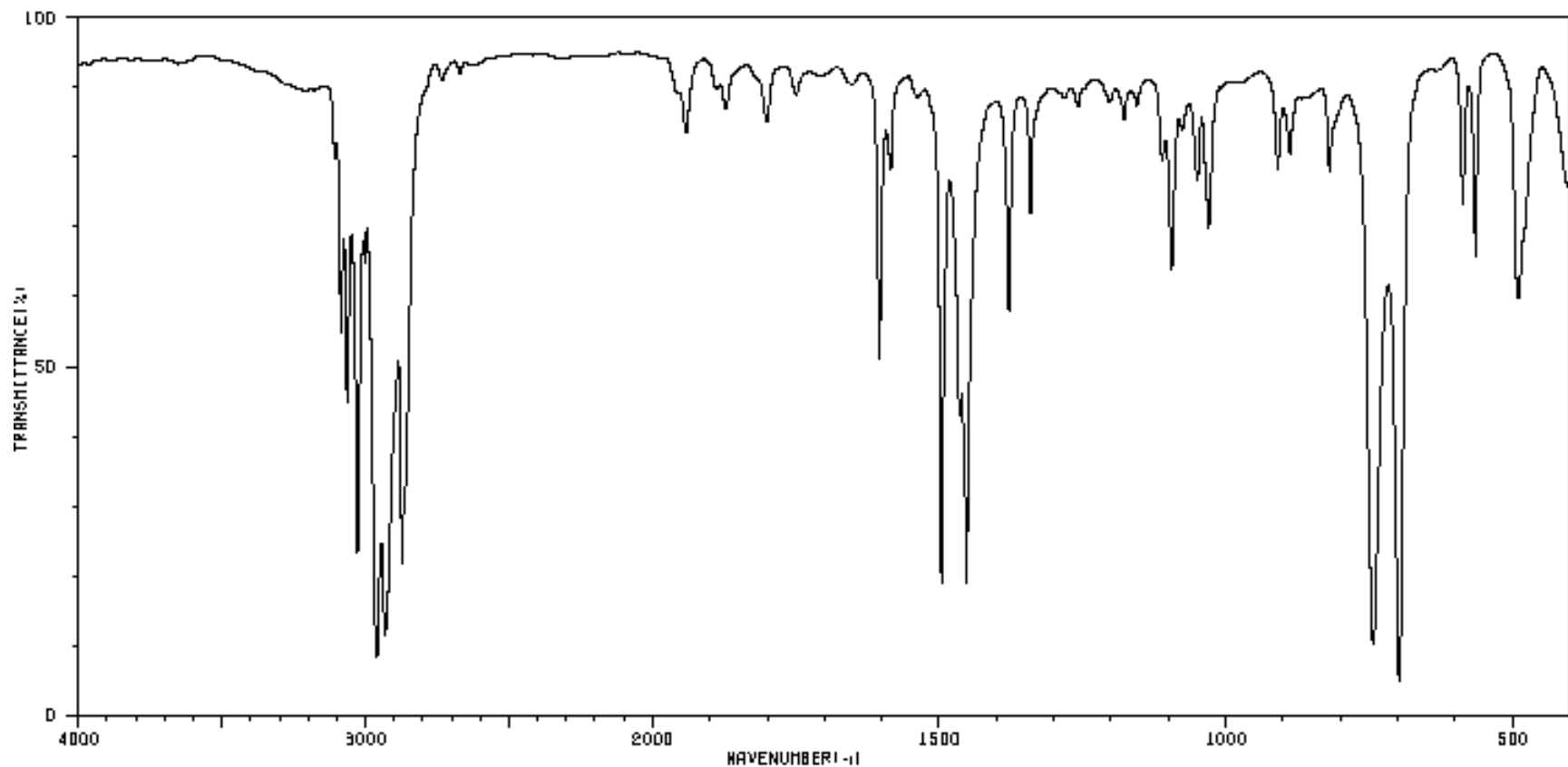


3084	62	2871	38	1466	42	1281	77	1028	44
3064	53	1942	84	1458	53	1213	84	922	81
3026	37	1858	85	1452	31	1150	85	905	79
3002	68	1800	84	1384	52	1144	86	761	9
2961	7	1604	62	1364	57	1108	81	699	4
2927	35	1583	84	1323	81	1082	62	535	54
2890	46	1494	28	1300	81	1050	57	478	84

isopropylbenzene

n-propylbenzene?

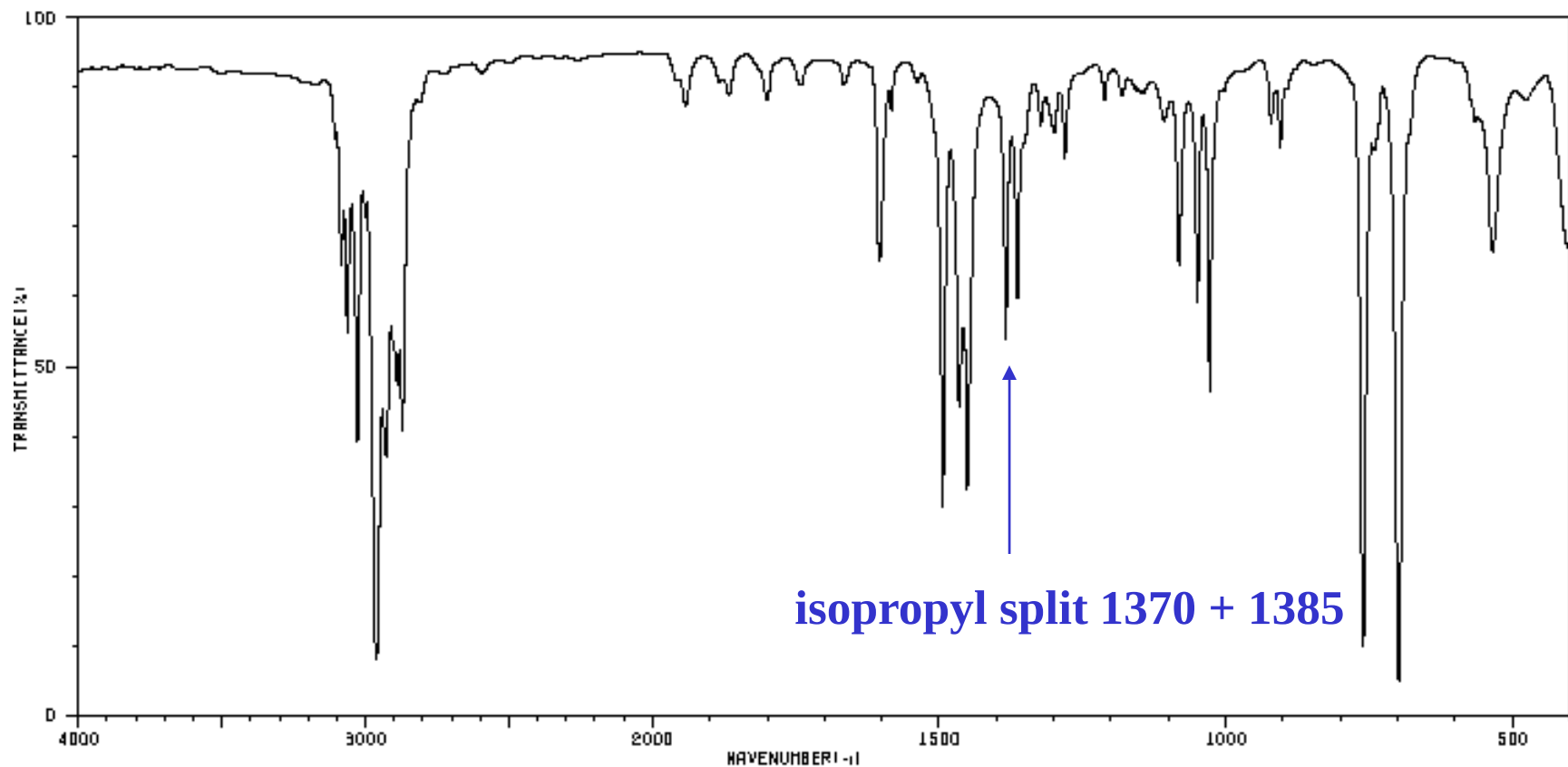
HIT-NO=1235	SCORE= ()	SDBS-NO=896	IR-NIDA-64858 : LIQUID FILM
PROPYL BENZENE <i>n</i> -propylbenzene			
C ₉ H ₁₂			



3108	77	2873	20	1466	41	1111	77	819	74
3085	52	1941	79	1453	18	1095	62	743	9
3064	43	1801	81	1379	55	1076	81	696	4
3028	22	1604	49	1341	70	1060	74	687	70
3002	62	1584	74	1258	84	1031	66	565	62
2960	8	1538	84	1203	84	909	74	490	57
2931	10	1496	18	1178	81	888	77	481	66

CCCC1=CC=CC=C1

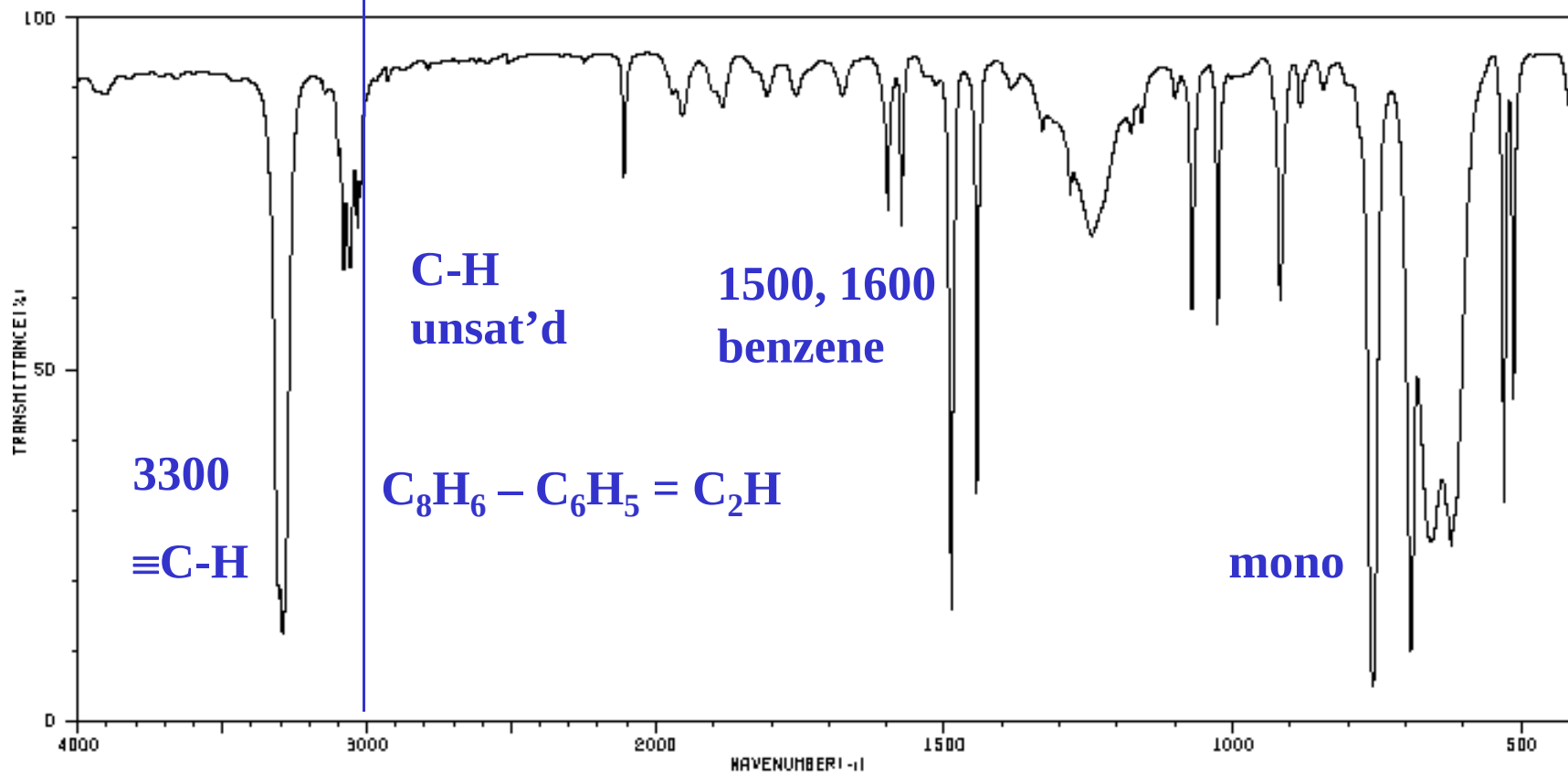
HIT-NO=1576	SCORE= ()	SDBS-NO=1816	IR-NIDA-63602 : LIQUID FILM
CUMENE			
isopropylbenzene			
C_9H_{12}			



3084	62	2871	38	1466	42	1281	77	1028	44
3064	53	1942	84	1458	53	1213	84	922	81
3028	37	1858	85	1452	31	1150	85	905	79
3002	68	1800	84	1384	52	1144	86	761	9
2961	7	1604	62	1364	57	1108	81	699	4
2927	35	1583	84	1323	81	1082	62	535	54
2890	46	1494	28	1300	81	1050	57	478	84

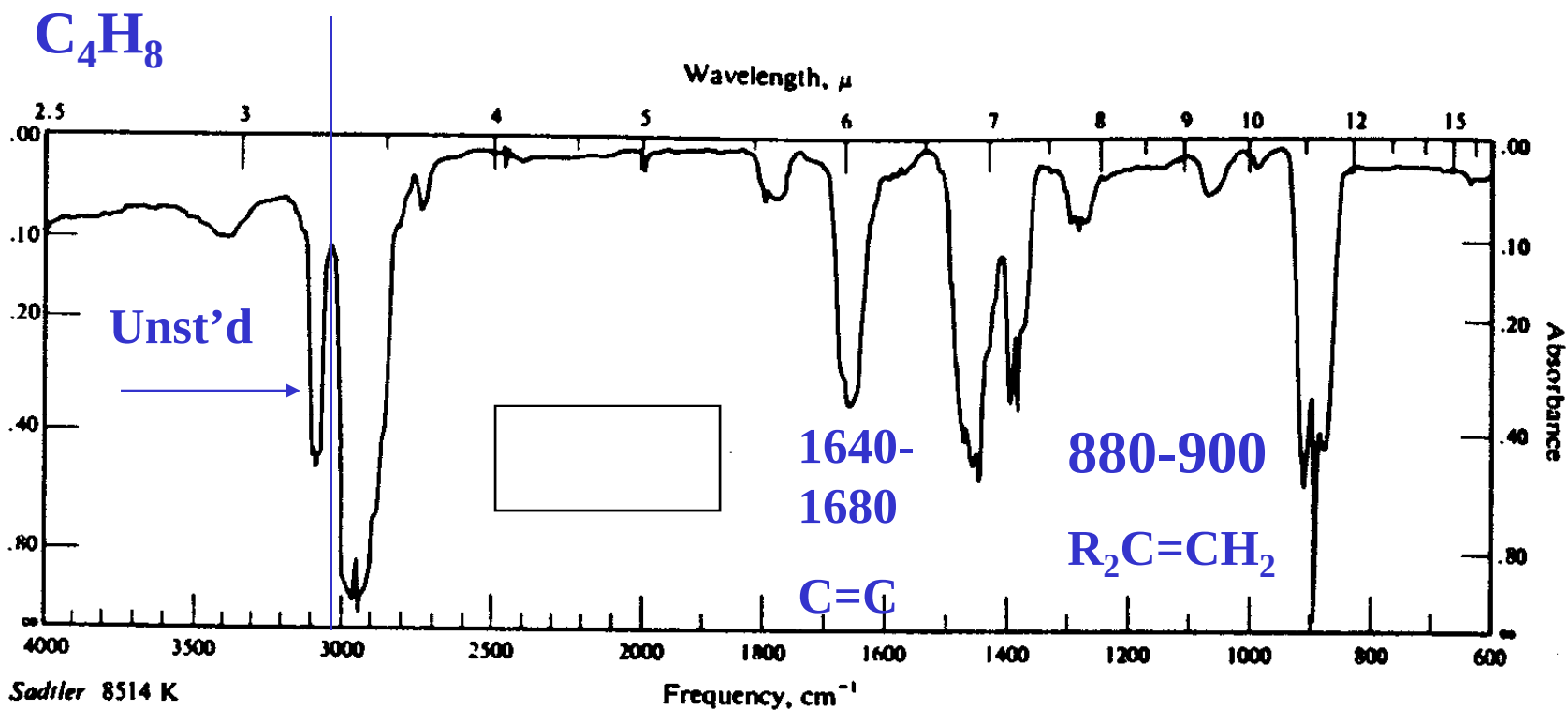
CC(C)c1ccccc1

HIT-NO=1445 SCORE= () SDBS-NO=1444 IR-NIDA-63379 : LIQUID FILM



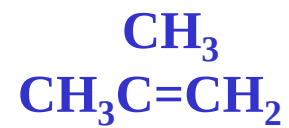
3906	86	2110	74	1674	68	1176	81	843	86
3306	16	1954	84	1488	15	1159	81	757	4
3291	12	1900	86	1444	31	1100	84	692	9
3081	62	1886	84	1386	86	1071	67	666	24
3058	62	1808	86	1331	81	1026	53	621	23
3034	86	1757	86	1282	72	918	57	530	30
3022	72	1698	70	1246	66	883	84	514	43

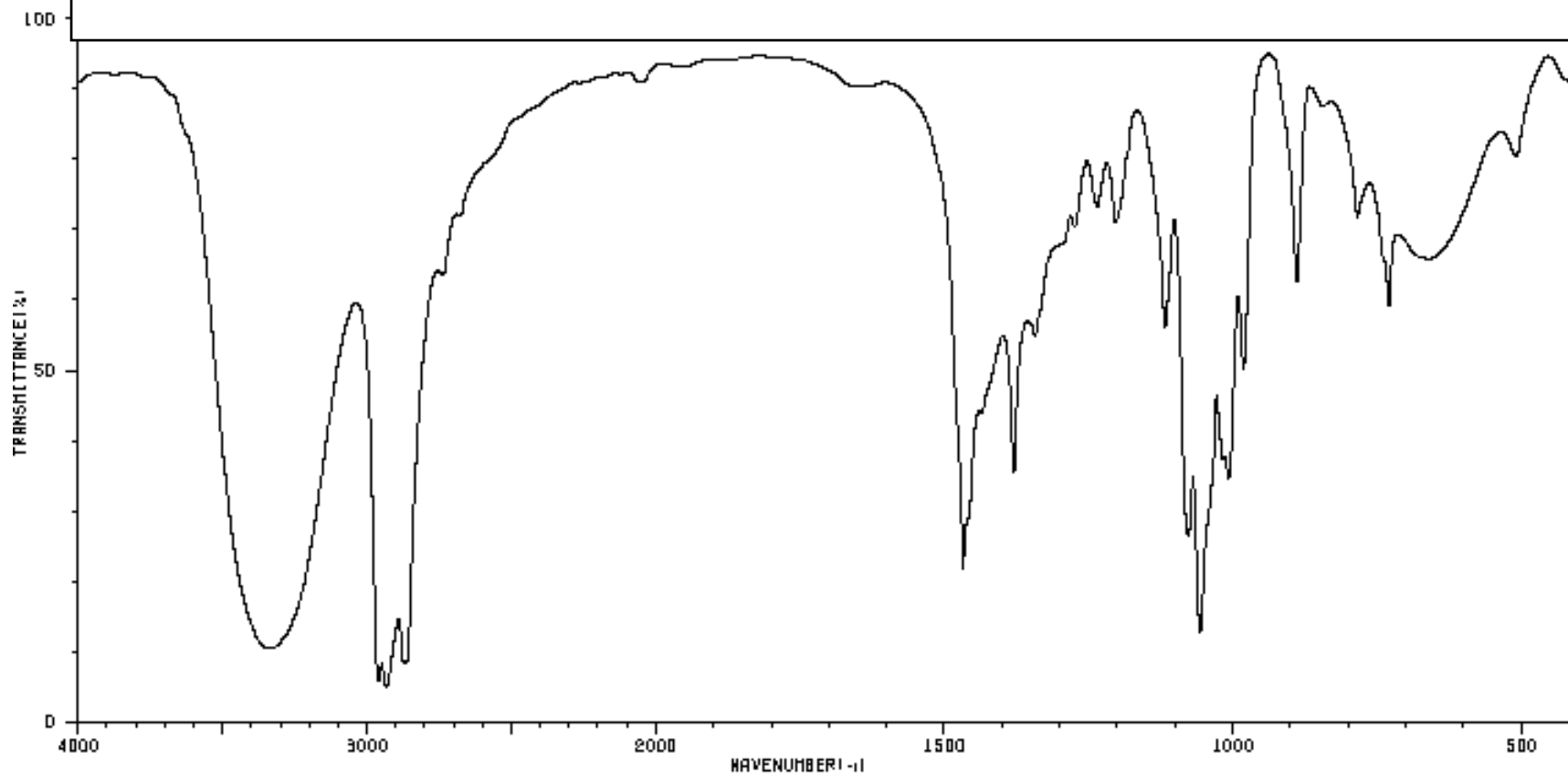
phenylacetylene



Wavelength, μ

isobutylene

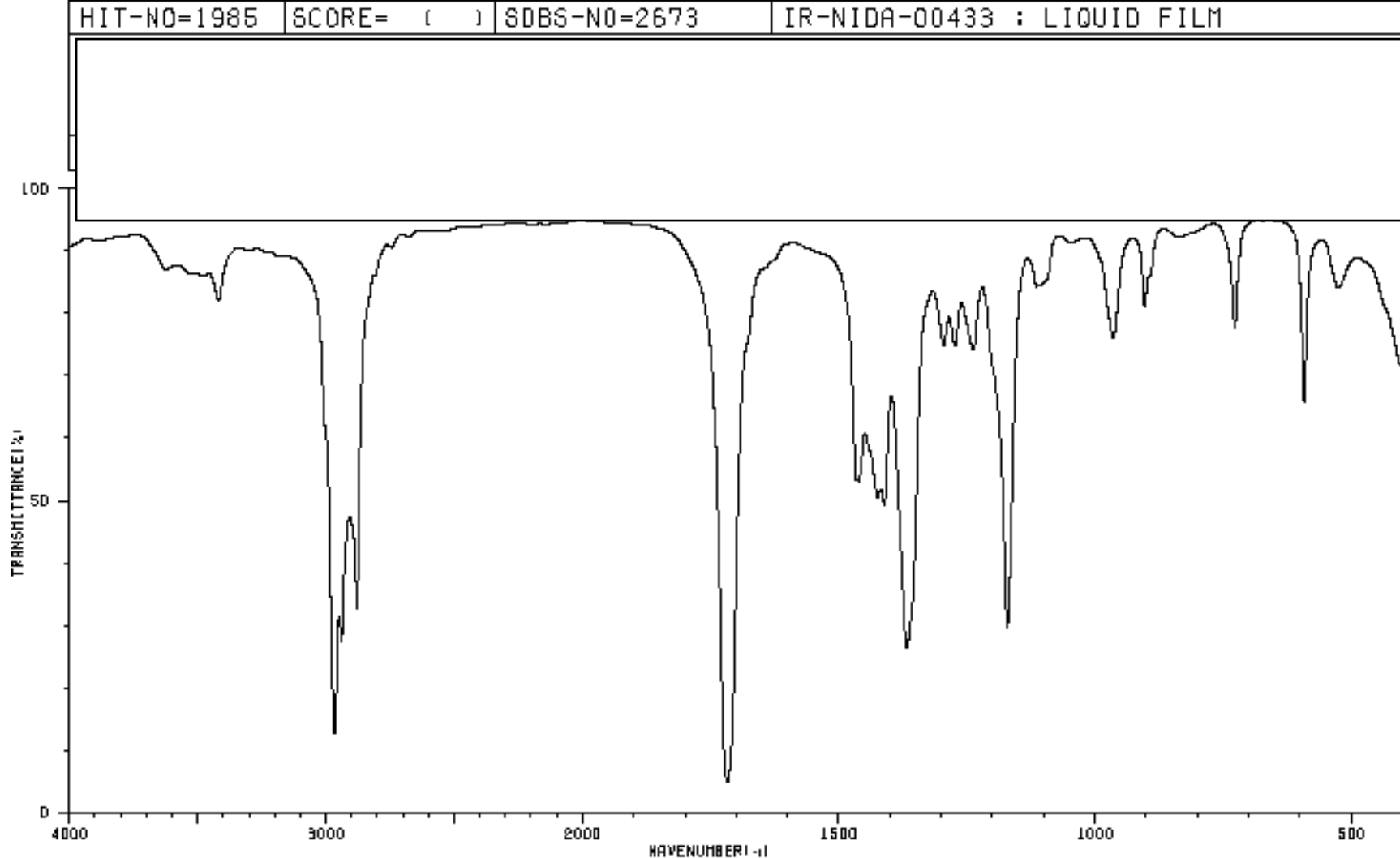




Which compound is this?

- a) 2-pentanone
- b) 1-pentanol
- c) 1-bromopentane
- d) 2-methylpentane

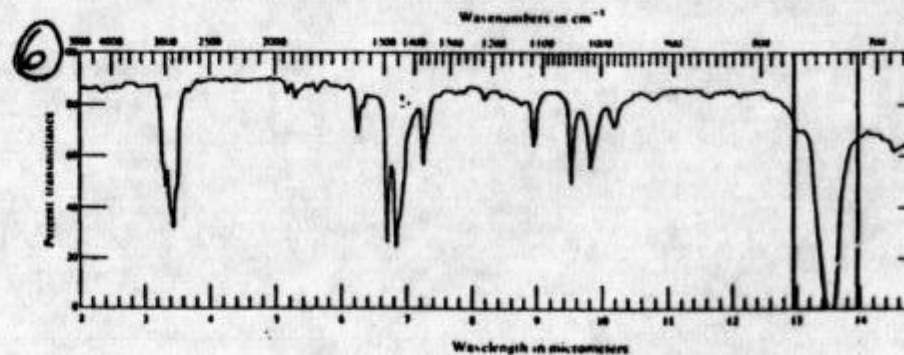
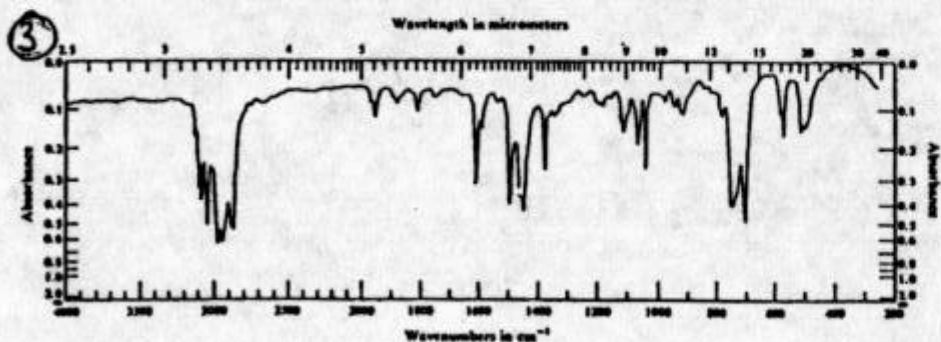
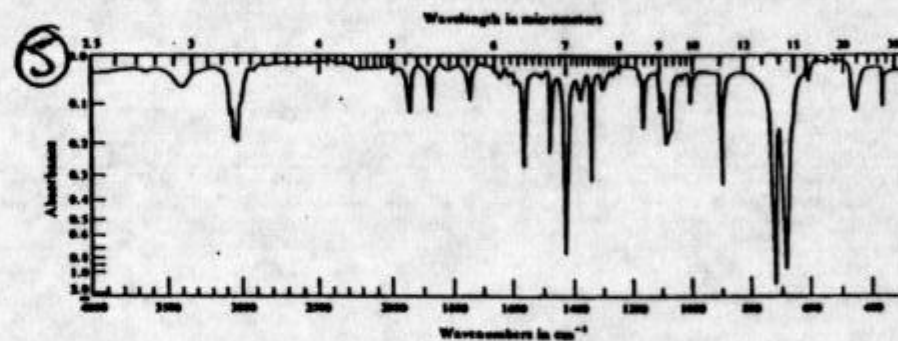
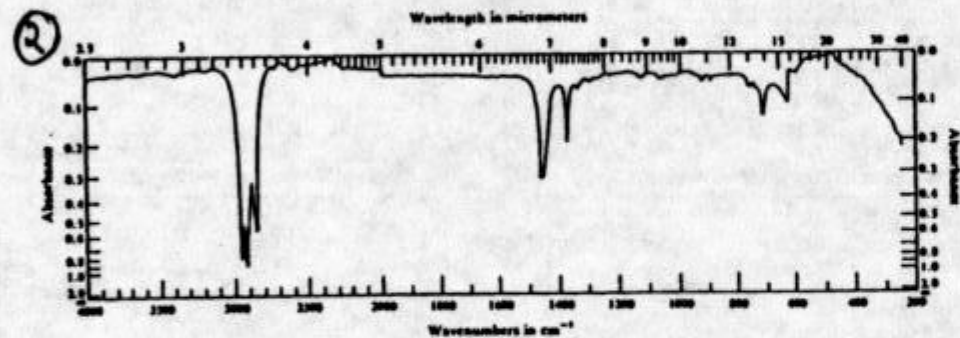
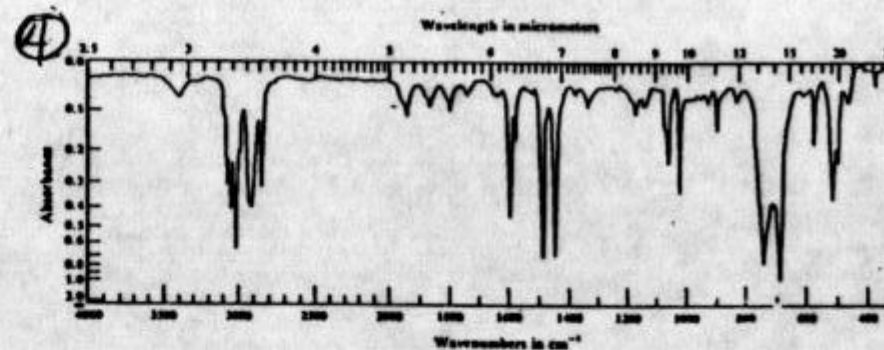
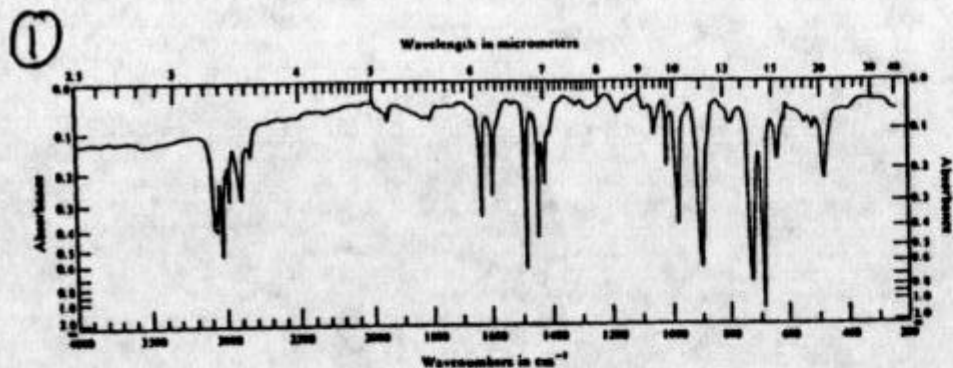
1-pentanol



What is the compound?

- a) 1-bromopentane
- b) 1-pentanol
- c) 2-pentanone
- d) 2-methylpentane

2-pentanone



A. biphenyl

B. o-xylene

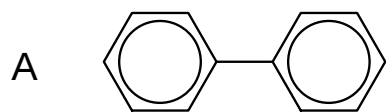
C. allylbenzene

D. n-pentane

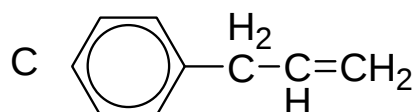
E. 1,2-diphenylethane

F. n-butylbenzene

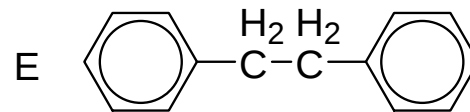
In a “matching” problem, do **not** try to fully analyze each spectrum. Look for differences in the possible compounds that will show up in an infrared spectrum.



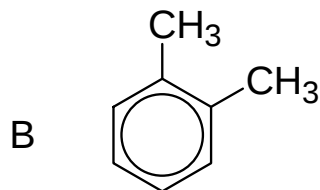
biphenyl



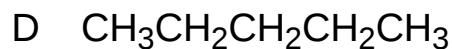
allylbenzene



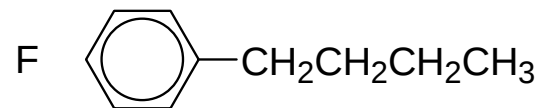
1,2-diphenylethane



o-xylene



n-pentane



n-butylbenzene

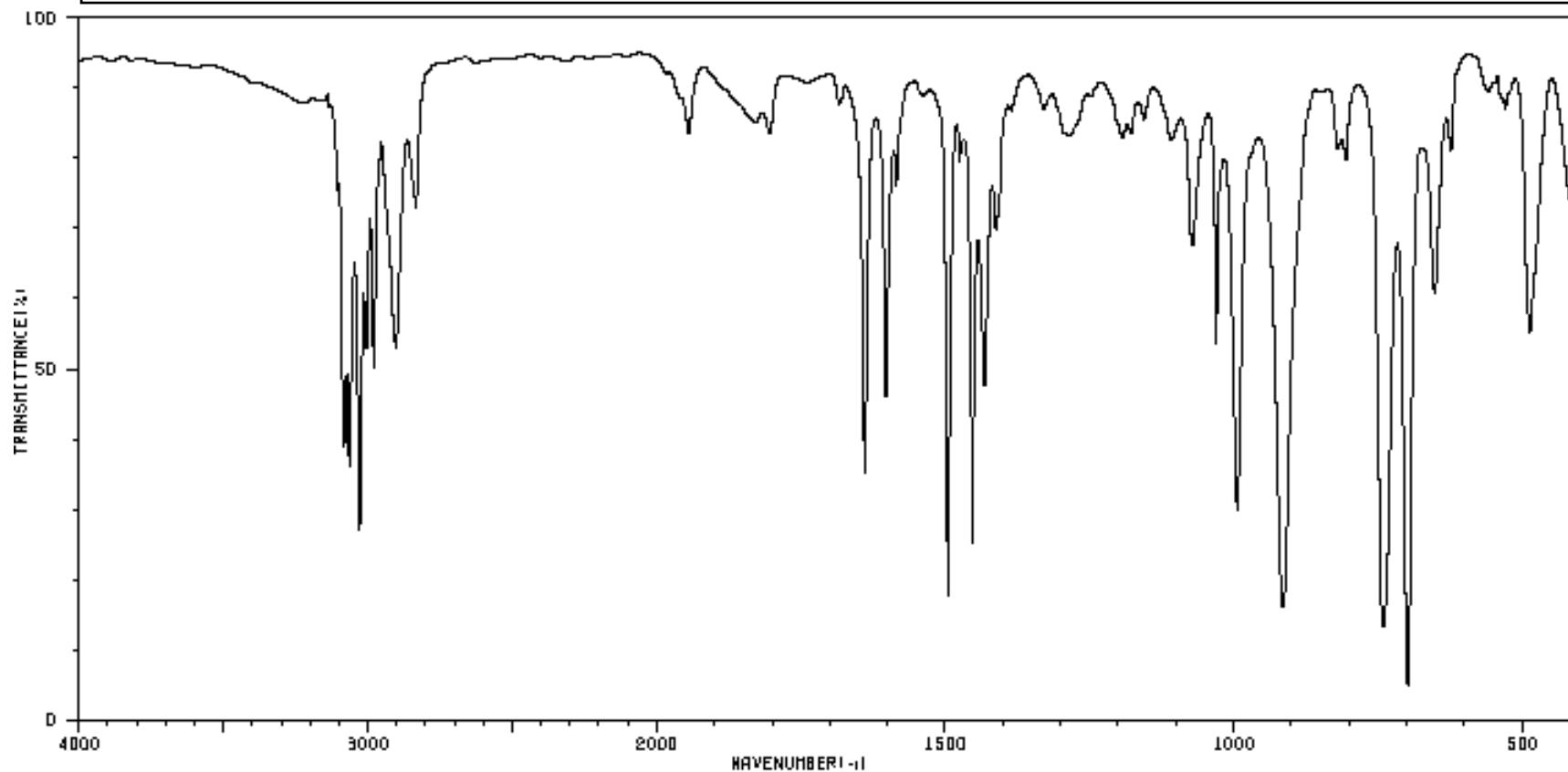
HIT-NO=3317

SCORE= ()

SDBS-NO=6325

IR-NIDA-64189 : LIQUID FILM

1



3082	37	1946	81	1463	24	1107	79	806	77
3064	34	1804	79	1432	46	1071	64	741	13
3029	26	1639	34	1412	86	1030	52	699	4
3006	50	1603	44	1286	79	994	28	662	58
2979	49	1585	72	1194	79	914	15	625	79
2904	50	1495	17	1186	81	821	79	487	53
2833	70	1476	77	1178	81	816	78	481	58

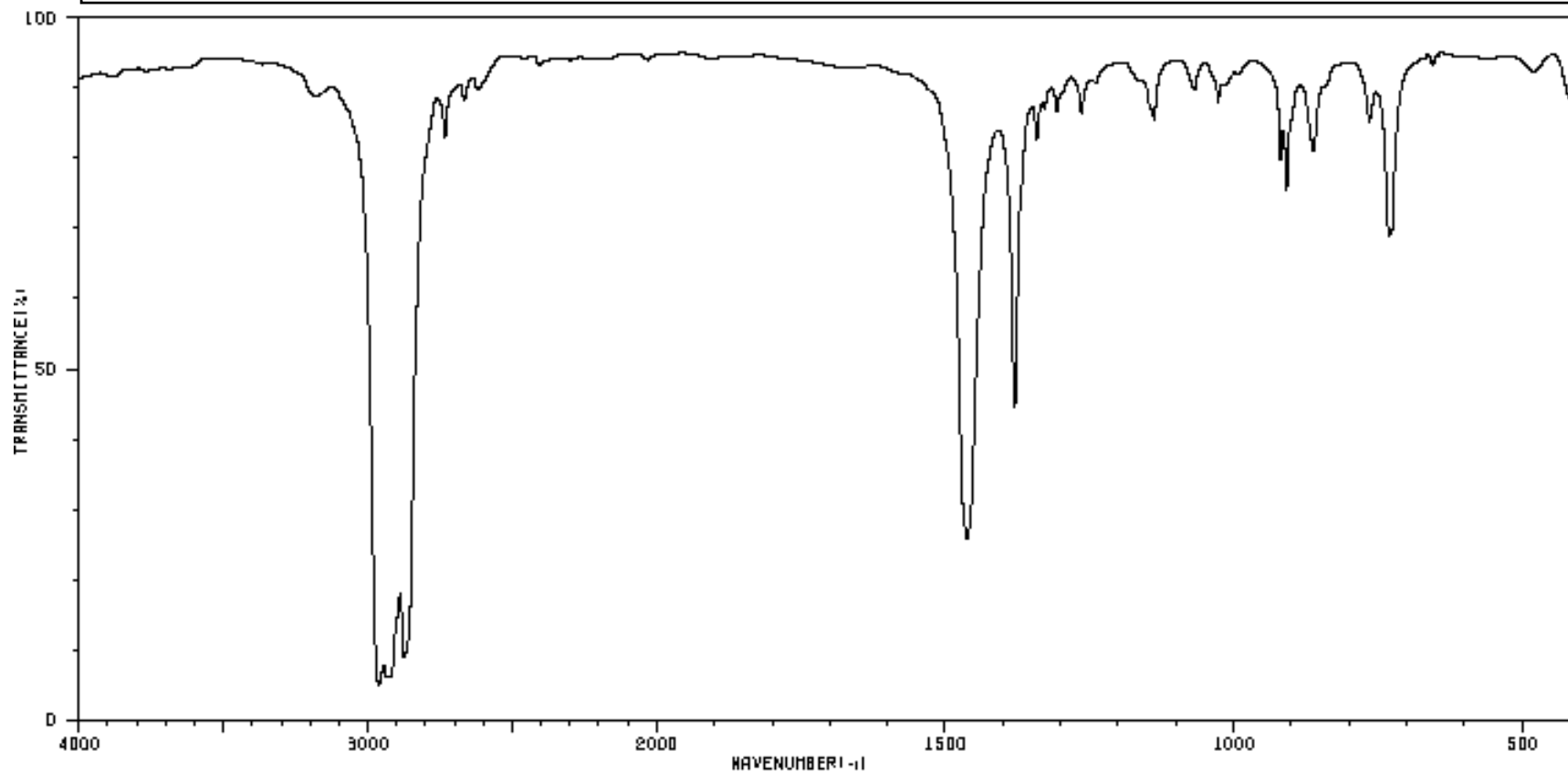
HIT-NO=1929

SCORE= ()

SDBS-NO=2475

IR-NIDA-68185 : LIQUID FILM

2



3182	86	2619	86	1138	81	732	66
3172	86	1462	24	1068	86		
2961	4	1380	45	1027	84		
2928	6	1342	79	919	77		
2875	8	1307	84	908	72		
2733	79	1264	84	862	79		
2666	84	1144	84	766	81		

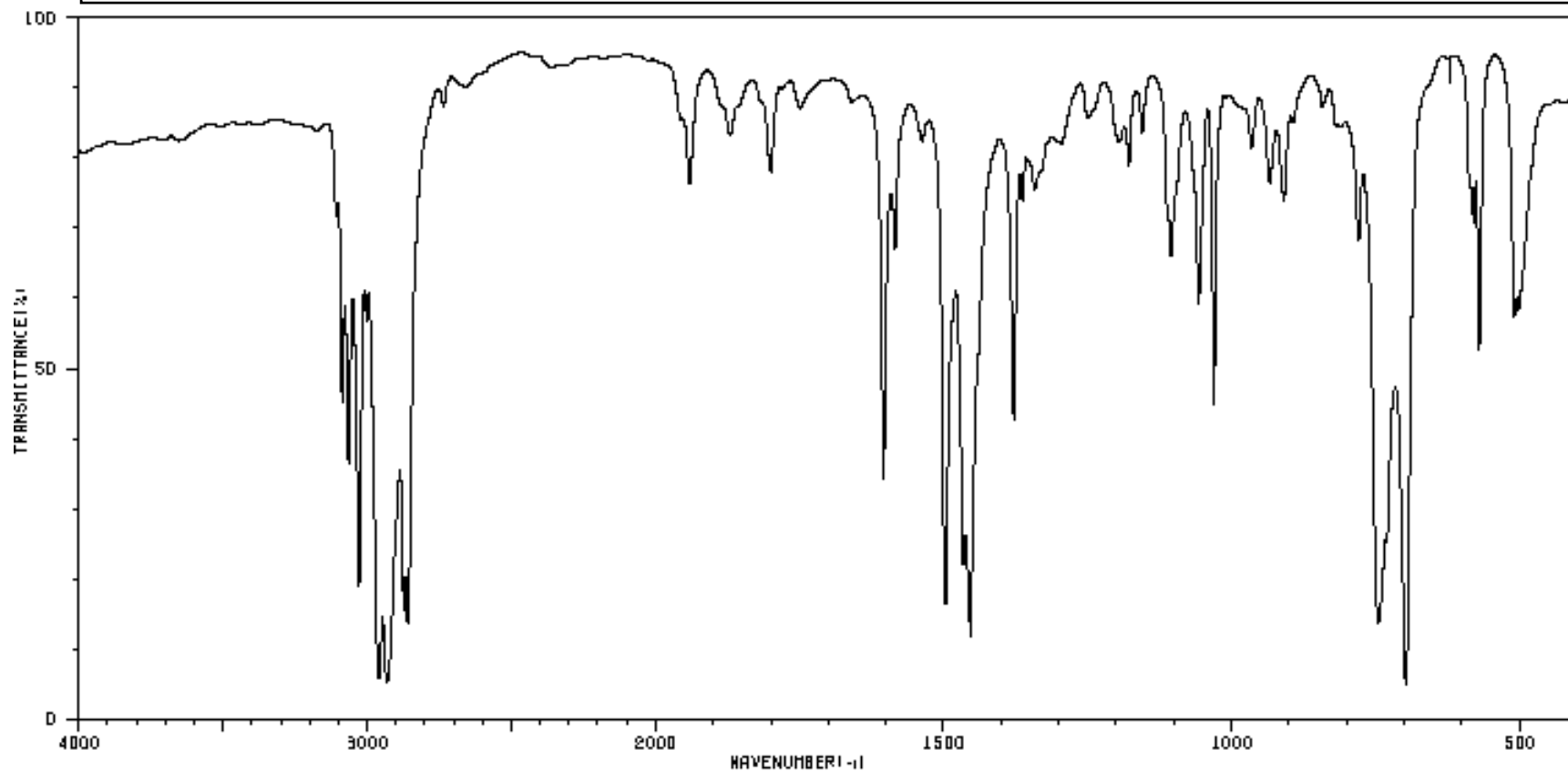
HIT-NO=1575

SCORE= ()

SDBS-NO=1815

IR-NIDA-02821 : LIQUID FILM

3



3108	68	2873	14	1467	21	1067	67	731	23
3087	43	2860	13	1454	11	1030	43	698	4
3064	35	1941	74	1379	41	965	79	588	72
3028	18	1800	74	1363	70	934	74	581	68
3002	55	1604	33	1342	72	909	70	570	50
2958	5	1584	64	1179	77	779	66	510	55
2931	4	1497	16	1106	64	746	19	503	67

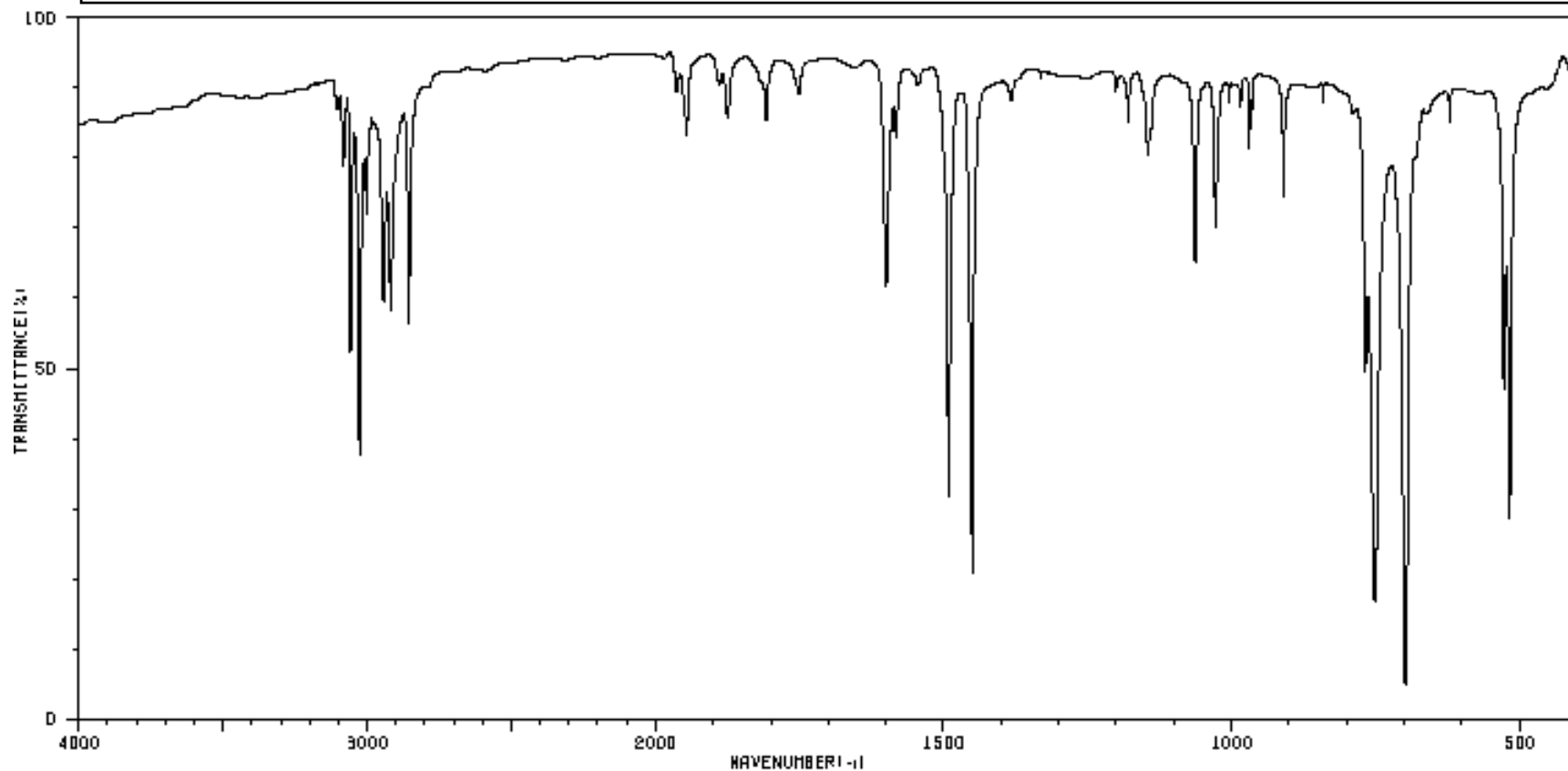
HIT-NO=1384

SCORE= ()

SDBS-NO=1264

IR-NIDA-62151 : KBR DISC

4



3102	84	2919	56	1600	58	1146	77	841	84
3083	77	2856	55	1583	79	1064	62	768	47
3056	50	1953	86	1492	30	1028	68	752	16
3040	79	1946	79	1460	20	1003	84	699	4
3027	36	1874	81	1383	84	985	84	622	81
3002	66	1808	81	1202	86	969	79	526	44
2943	57	1761	86	1180	81	910	72	518	27

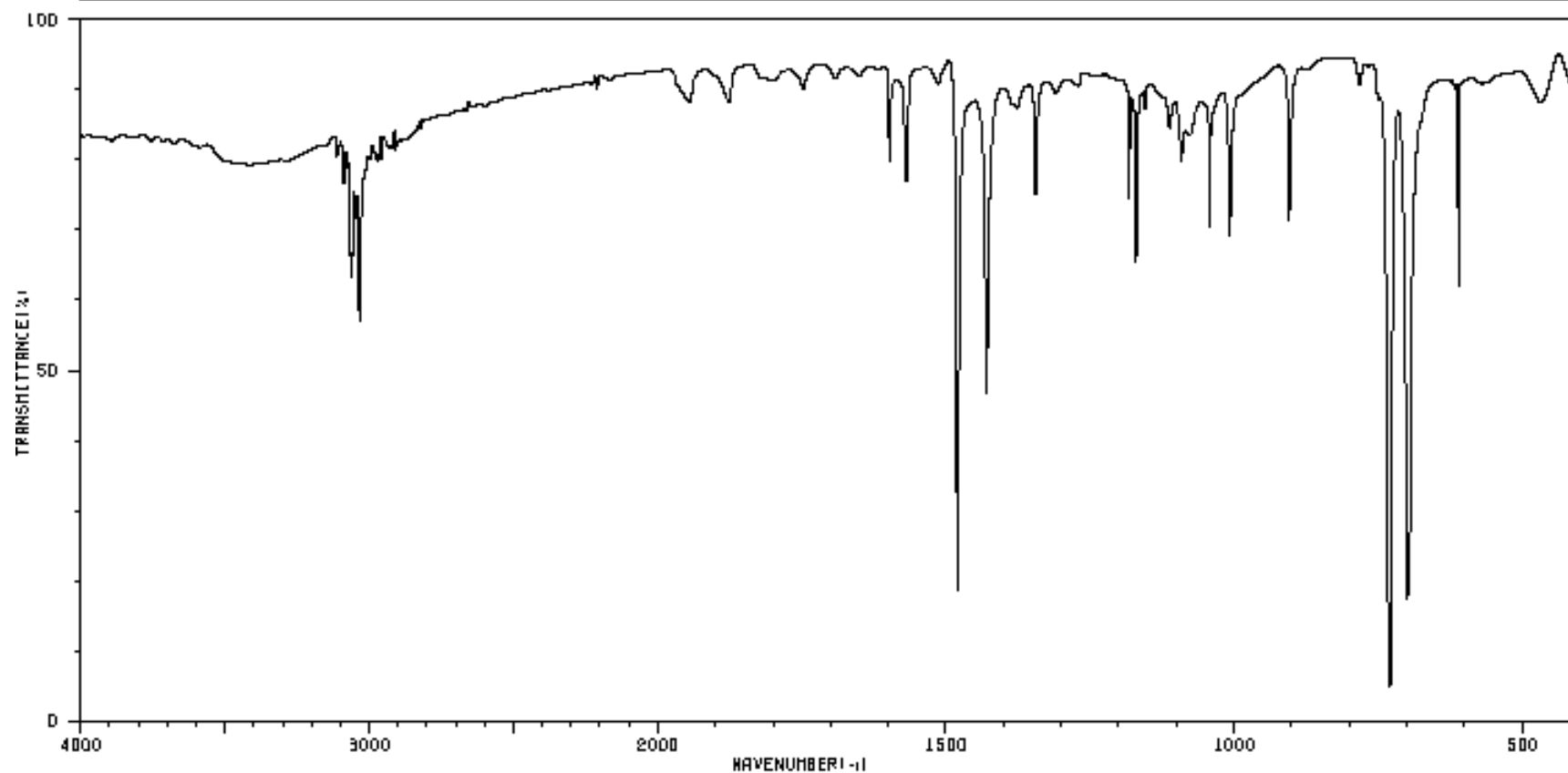
HIT-NO=1355

SCORE= ()

SDBS-NO=1182

IR-NIDA-60114 : KBR DISC

5



3111	77	2934	79	1669	74	1183	72	1007	66
3088	74	2921	79	1481	18	1170	62	904	68
3064	80	2908	79	1430	44	1155	84	730	4
3046	68	2876	79	1386	84	1112	81	700	16
3035	55	1944	84	1377	84	1092	77	611	60
2970	77	1877	84	1345	72	1077	79	466	64
2959	77	1699	77	1309	86	1043	68		

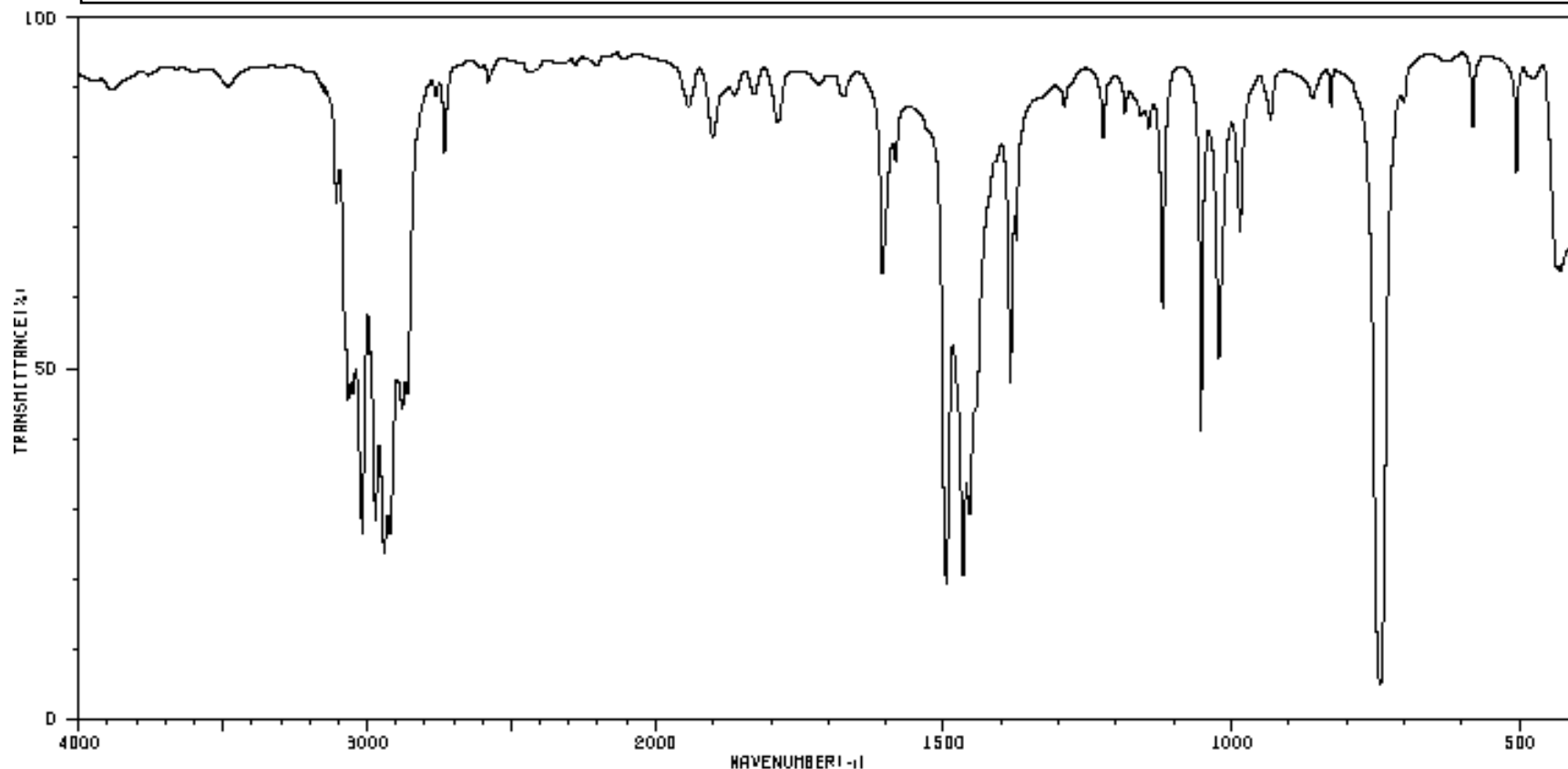
HIT-NO=1272

SCORE= ()

SDBS-NO=1028

IR-NIDA-21942 : LIQUID FILM

6



3108	70	2878	42	1683	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	48	431	62