The Infra-Red Spectra of the Isomeric Octanes in the Liquid Phase*

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(Received January 15, 1943)

IN recent years, industry has become interested in the use of infra-red spectroscopy as an analytical tool. This is because the infra-red spectra of related compounds show differences, often quite marked, while the other physical and chemical properties are so similar that it is impossible to distinguish between the compounds readily. It has been stated by Nielsen[1] that infra-red spectra may be used to distinguish between any two compounds except between enantiomorphic stereoisomers. To use infra-red spectra for analyses, in general it is necessary to have available the spectra of pure samples of the substances in question. It is one of the purposes of this investigation to present infra-red spectroscopic data which may serve as standards for analytical purposes.

A second purpose of this investigation is that of providing data which may be useful in the study of molecular structure. For a number of years, theoretical physicists have been making use of infra-red spectra of relatively simple molecules to determine molecular structure. Because of the greatly increased complexity of the problem, little has been done to date in the correlation of infra-red spectra of complex molecules with their structure. It is the hope of the authors that the spectra of this group of similar molecules which are of intermediate size, may provide data which will assist in making the transition from the simpler to the more complex molecules. Work on the interpretation of these spectra is in fact now under way in this laboratory. These data may possibly be useful also in

TABLE I. Physical properties of isomeric octanes for which infra-red spectra are obtained.

A.P.I. No.	Compound	Melting Point °C	Boiling Point °C	Specific Gravity S.G.$_4^{20}$	Index of Refraction n_D^{20}	Impurities: Halides	Olefins	Moisture	Isomeric Octanes
6-P	*n*-Octane	−56.90	125.6	0.7019	1.3976	none	none	trace ?	
5-P	2-Methylheptane	−109.63	118.0; 118.2	0.6976	1.3955	none	none	trace ?	3,3-Dimethylhexane possible
4-P	3-Methylheptane	−120.80	119.1	0.7055	1.3988	none	none	trace ?	*n*-octane possible
3-P	4-Methylheptane	−121.09	117.5	0.7042	1.3980	none	none	trace ?	
29-BL	2,2-Dimethylhexane	glass	107.1	0.6954	1.3940	none	none	trace ?	2,3,-Dimethylhexane probable (b. pts. wide)
16-BL	2,3-Dimethylhexane	glassy	115.5	0.7125	1.4020	none	none	trace ?	2,2-Dimethylhexane (b. pts. wide) and 3,3-Dimethylhexane possible (b. pts. medium spread)
12-BL	2,4-Dimethylhexane	glassy	109.8	0.7002	1.3958	none	none	trace ?	2,5-Dimethylhexane possible (b. pts. close)
7-P	2,5-Dimethylhexane	−91.49	109.3	0.6939	1.3929	none	none	trace ?	
33-BL	3,3-Dimethylhexane	glass	111.9	0.7103	1.4007	none	none	trace ?	3,4-Dimethylhexane probable (b. pts. wide) 2-methyl-3-ethylpentane possible (b. pts. medium spread)
20-BL	3,4-Dimethylhexane	glass	118.0	0.7185	1.4041	none	none	trace ?	
8-BL	3-Ethylhexane	glassy	118.7	0.7128	1.4021	none	none	trace ?	4-Methylheptane possible (b. pts. close)
36-BL	2,2,3-Trimethylpentane	−113.3	110.0	0.7156	1.4029	none	none	trace ?	2,3,3-Trimethylpentane probable (b. pts. medium spread)
31-P	2,2,4-Trimethylpentane	−107.40	99.4	0.6916_6	1.3918	none	none	trace ?	
27-BL	2,3,3-Trimethylpentane	−102.4	114.7	0.7258_1	1.4079	none	none	trace ?	2,2,3-Trimethylpentane probable (b. pts. medium spread)
9-P	2,3,4-Trimethylpentane	−109.32	113.8	0.7182	1.4045	none	none	trace ?	
17-BL	2-Methyl-3-ethylpentane	−116.3	115.7	0.7191	1.4046	none	none	trace ?	3,3-Dimethylhexane possible (b. pts. medium spread)
35-BL	3-Methyl-3-ethylpentane	−89.7	118.5	0.7272	1.4079	none	none	trace ?	
40-BL	2,2,3,3-Tetramethylbutane	+101	106.5 to 106.6	solid	solid	none	none	trace ?	

* Through the courtesy of the authors and of the editors of the Journal of Applied Physics we were permitted to include this paper in a symposium issue of the Reviews of Modern Physics. The paper had been originally set in type for the Journal of Applied Physics and was not presented at the symposium. It is one of three papers planned to report the work on the octanes. The first paper has already appeared in the Reviews of Scientific Instruments **13**, 515 (1942). The third paper is published immediately following this one.

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[1] J. R. Nielsen, Oil and Gas. J. **40**, 34 (1942).

TABLE II. Accuracy with which the location of sharp absorption lines may be determined.

Region		Accuracy	
Wave-Length	Frequency	Wave-Length	Frequency
15μ	667 cm^{-1}	0.002μ	0.09 cm^{-1}
5	2000	.005	2
2	5000	.01	25

the determination of thermodynamic quantities of these compounds.

HISTORICAL

The first known infra-red spectrum obtained of any of the isomeric octanes was that of liquid *n*-octane published by Coblentz[2] in 1905. Kettering and Sleator[3] published the spectrum of 2,2,4-trimethylpentane in the vapor phase in 1933. These two publications cover the spectral range from 1 to 15μ. In 1938, Lambert and Lecomte[4] obtained spectra of all octanes as liquids between 7 and 15μ. Two other papers present spectra of restricted regions at higher resolution. In the first of these, Meyer, Bronk, and Levin[5] covered the 3.5μ region of *n*-octane in 1927. Liddel and Kasper[6] obtained spectra of *n*-octane and 2,2,4-trimethylpentane between 1 and 2μ in 1933.

The results of this investigation present spectra of the eighteen isomeric octanes in the regions

TABLE III. Wave-lengths and wave numbers of the absorption lines in the infra-red spectra.

n-Octane			2-Methylheptane			3-Methylheptane			4-Methylheptane			2,2-Dimethylhexane		
Designation	Wave-length (μ)	Wave number (cm^{-1})	Designation	Wave-length (μ)	Wave number (cm^{-1})	Designation	Wave-length (μ)	Wave number (cm^{-1})	Designation	Wave-length (μ)	Wave number (cm^{-1})	Designation	Wave-length (μ)	Wave number (cm^{-1})
O_1	1.709	5851	A	1.697	5893	A	1.703	5872	A	1.710	5848	A	1.704	5869
O_2	1.747	5724	B	2.319	4312	B	2.317	4316	B	2.322	4307	B	2.322	4307
A	2.314	4322	C	2.453	4077	B_a	2.344	4266	B_a	2.356	4244	C	2.420	4132
A_a	2.343	4268	C_a	2.621	3815	C	2.454	4075	C	2.450	4082	C_a	2.618	3820
A_b	2.391	4182	C_b*	2.780	3597	D	2.606	3837	C_a	2.580	3876	D*	2.778	3600
B	2.443	4093	C_c	2.975	3361	E*	2.788	3587	C_b	2.677	3736	D_a	2.960	3378
B_b*	2.776	3602	D	3.150	3175	E_a	2.960	3378	D*	2.785	3591	E	3.121	3204
B_c	2.949	3391	E_1	3.420	2924	F	3.155	3170	E	3.142	3183	F_1	3.414	2929
C	3.127	3198	E_2	3.487	2868	G_1	3.421	2923	F_1	3.415	2928	F_2	3.479	2874
D_1	3.422	2922	F	3.670	2725	G_2	3.488	2867	F_2	3.483	2871	H	3.686	2713
D_2	3.493	2863	G	3.837	2606	H	3.665	2729	G	3.674	2722	H_a	3.762	2658
E	3.660	2732	H	4.235	2361	H_a	3.743	2672	H	3.826	2614	H_b	3.819	2618
F	3.751	2666	J	6.812	1468	J	3.844	2601	J	4.001	2499	J	3.911	2557
F_a	3.814	2622	K_1	7.222	1385	J_a	4.259	2348	J_a	4.189	2387	J_a	4.232	2363
G	3.853	2595	K_2	7.306	1369	K	6.831	1464	J_b	4.284	2334	J_b	4.370	2288
G_a	3.975	2516	L	7.460	1340	L	7.246	1380	J_c	4.609	2170	J_c	4.760	2101
G_b	4.155	2407	M	7.666	1304	M	7.382	1355	J_d	4.911	2036	L	6.808	1469
G_c	4.299	2326	N	7.815	1280	M_a	7.583	1319	J_e	5.255	1903	N	7.041	1420
G_d	4.927	2030	P	8.059	1241	N	7.684	1301	K_1	6.812	1468	P	7.176	1394
H	6.813	1468	Q	8.270	1209	P	7.857	1273	K_2	6.854	1459	Q	7.245	1380
H_a	7.034	1422	R	8.528	1173	Q	8.007	1249	L	7.242	1381	R	7.320	1366
J	7.242	1381	S	8.741	1144	R	8.225	1216	M	7.450	1342	S	7.457	1341
J_a	7.371	1357	T	9.211	1086	R_a	8.368	1195	M_a	7.672	1303	T_1	7.602	1315
K	7.440	1344	U_1	9.563	1046	S_1	8.668	1154	N_1	7.790	1284	T_2	7.679	1302
L	7.677	1303	V	10.386	963	S_2	8.736	1145	N_2	7.866	1271	T_a	7.876	1270
M	7.861	1272	V_a	10.533	949	S_a	8.860	1129	P	7.998	1250	U	7.988	1252
N	8.154	1226	W_1	10.720	933	S_b	8.994	1112	Q	8.182	1222	V	8.309	1204
P	8.346	1198	W_2	10.882	919	T	9.253	1081	Q_b	8.528	1173	V_a	8.725	1146
Q	8.802	1136	W_a	11.007	909	T_a	9.393	1065	R_1	8.648	1156	V_b	8.866	1128
R_1	9.224	1084	X	11.186	894	T_b	9.578	1044	R_2	8.732	1146	W_1	9.054	1104
R_2	9.284	1077	Y	11.930	838	U_1	9.878	1012	S	9.302	1075	W_2	9.143	1094
R_a	9.719	1029	Y_a	12.109	826	U_2	10.007	999	S_a	9.543	1048	X	9.370	1067
R_b	9.910	1009	Y_b	12.284	814	V	10.369	964	S_b	9.672	1034	X_a	9.703	1031
S	10.330	968	Z	13.027	768	V_a	10.772	928	S_c	9.882	1012	Y	9.879	1012
T	10.912	916	Z_a	13.248	755	W_1	11.010	908	S_d	10.092	991	Y_a	10.290	972
T_a	11.081	902	AA	13.792	725	W_2	11.170	895	T	10.482	954	Y_b	10.747	930
T_b	11.188	894				W_a	11.420	876	T_a	10.959	912	Y_c	10.889	918
U	11.378	879				W_b	12.179	821	T_b	11.037	906	Y_d	10.985	910
V	11.834	845				X_1	12.801	781	T_c	11.225	891	Y_e	11.039	906
V_a	12.584	795				X_2	12.964	771	T_d	11.474	872	Z	11.184	894
W	13.063	766				X_3	13.122	762	T_f	11.978	834	Z_a	11.422	876
W_a	13.329	750				Y	13.737	728	T_g	12.124	824	AA	12.724	786
W_b	13.614	735				Z	14.544	688	T_h	13.101	763	AA_a	13.169	759
X	13.841	722							U	13.513	740	BB	13.706	730

* Probably due to impurity in sodium chloride prism.

[2] W. W. Coblentz, *Investigations of Infrared Spectra* (Carnegie Institute Publication No. 35, 1905), p. 217.

[3] C. F. Kettering and W. W. Sleator, Physics **4**, 47 (1933).

[4] P. Lambert and J. Lecomte, Ann. de physique [2] **10**, 524 (1938).

[5] C. F. Meyer, D. W. Bronk, and A. A. Levin, J. Opt. Soc. Am. **15**, 257 (1927).

[6] U. Liddel and C. Kasper, Bur. Stand. J. Research **11**, 599 (1933).

between 1.5 and 15μ. Data for the liquid phase* are given in this paper and for the vapor phase in the paper which follows this.[7]

PURITY OF SAMPLES

Table I contains some physical properties of the samples used in this research as furnished by the American Petroleum Institute. The first column gives the designation of the A. P. I. Hydrocarbon Research Project. The melting and boiling points are those reduced to a pressure of 1 atmosphere. The specific gravity is that of the substance at 20°C compared to water at 4°C. The index of refraction is that of the substance at 20°C for the sodium D line.

APPARATUS

A description of the spectrograph used, operating techniques employed, and accuracy of the instrument are given in another paper.[8] For the present purpose, the following brief description is given. A 60° sodium chloride prism with sides 8 cm by 10 cm is used with a Wadsworth-Littrow arrangement of mirrors. The collimating mirror has a focal length of 50 cm. The entire spectrograph and source housing is evacuable. A Nernst

TABLE III.—*Continued.*

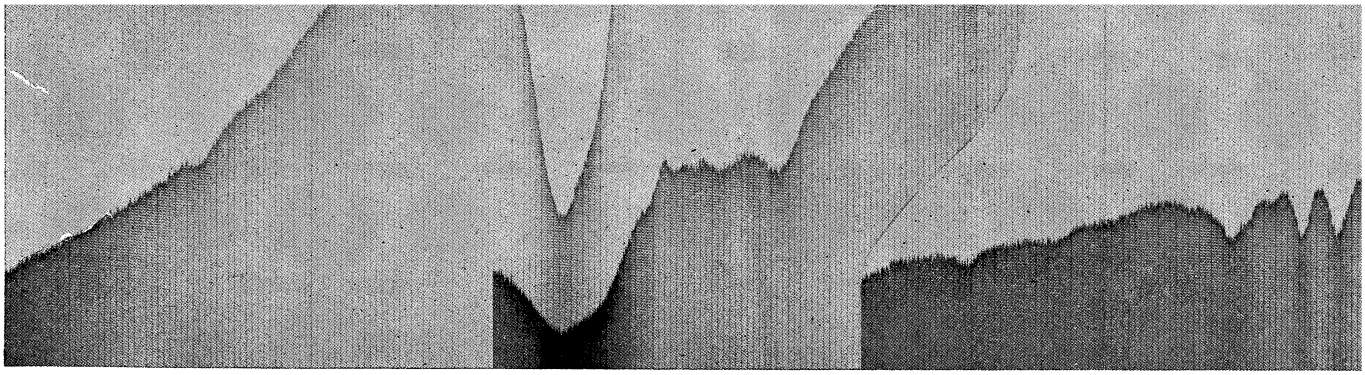
2,3-Dimethylhexane			2,4-Dimethylhexane			2,5-Dimethylhexane			3,3-Dimethylhexane			3,4-Dimethylhexane		
Designation	Wavelength (μ)	Wave number (cm^{-1})	Designation	Wavelength (μ)	Wave number (cm^{-1})	Designation	Wavelength (μ)	Wave number (cm^{-1})	Designation	Wavelength (μ)	Wave number (cm^{-1})	Designation	Wavelength (μ)	Wave number (cm^{-1})
A	1.698	5889	A	1.705	5865	A	1.705	5865	A	1.697	5893	A	1.714	5834
B	2.321	4308	B	2.320	4310	B	2.320	4310	C	2.318	4314	B	2.317	4316
C	2.460	4065	C	2.464	4058	C	2.457	4070	D	2.406	4156	C	2.457	4070
Ca*	2.780	3597	Ca	2.614	3826	D	2.623	3812	Da	2.456	4072	D	2.597	3851
Cb	2.938	3404	D*	2.783	3593	E*	2.787	3588	E*	2.788	3587	E*	2.776	3602
D	3.154	3171	E	2.952	3388	F	2.980	3356	Ea	2.914	3432	Ea	2.942	3399
$E1$	3.409	2933	F	3.145	3180	G	3.149	3176	F	3.136	3189	F	3.163	3162
$E2$	3.478	2875	$G1$	3.422	2922	$H1$	3.415	2928	$G1$	3.409	2933	$G1$	3.405	2937
G	3.669	2726	$G2$	3.475	2878	$H2$	3.487	2868	$G2$	3.478	2875	$G2$	3.476	2877
Ga	3.746	2670	J	3.677	2720	J	3.677	2720	J	3.668	2726	H	3.665	2729
H	3.852	2596	K	3.874	2581	K	3.838	2606	K	3.786	2641	J	3.849	2598
Ha	4.203	2379	Ka	4.167	2400	Ka	4.003	2498	L	3.930	2545	K	4.167	2400
$K1$	6.815	1467	M	6.821	1466	Kb	4.053	2467	M	4.187	2388	Ka	4.274	2340
$K2$	6.853	1459	Q	7.036	1421	L	4.222	2369	P	6.820	1466	L	6.048	1653
$N1$	7.214	1386	R	7.227	1384	La	4.379	2284	$S1$	7.213	1386	M	6.828	1465
$N2$	7.243	1381	S	7.307	1369	M	6.807	1470	$S2$	7.241	1381	N	7.233	1383
$N3$	7.302	1369	T	7.463	1340	$N1$	7.214	1386	T	7.320	1366	$P1$	7.562	1322
P	7.488	1336	$U1$	7.694	1300	$N2$	7.300	1370	Ta	7.434	1345	$P2$	7.653	1307
Q	7.627	1311	$U2$	7.784	1285	P	7.465	1340	$U1$	7.581	1319	Pa	7.732	1293
Qa	7.710	1297	Ua	8.093	1236	Pa	7.586	1318	$U2$	7.636	1310	Q	7.865	1271
R	7.884	1268	V	8.533	1172	Q	7.721	1295	$U3$	7.698	1299	R	8.069	1239
Ra	7.978	1253	W	8.693	1150	R	7.920	1263	$U4$	7.775	1286	Ra	8.459	1182
S	8.102	1234	X	9.223	1084	S	8.161	1225	V	7.915	1263	Rb	8.607	1162
T	8.434	1186	Y	9.551	1047	T	8.531	1172	Va	8.113	1233	S	8.912	1122
U	8.718	1147	Ya	9.635	1038	U	9.166	1091	$W1$	8.240	1214	$T1$	9.335	1071
V	8.872	1127	Yb	9.866	1014	$V1$	9.552	1047	$W2$	8.395	1191	$T2$	9.400	1064
W	9.295	1076	Z	10.041	996	$V2$	9.635	1038	Wa	8.899	1124	Ta	9.527	1050
Wa	9.506	1052	AA	10.304	970	Va	10.396	962	$X1$	9.086	1101	$U1$	9.861	1014
X	9.678	1033	AAa	10.445	957	W	10.528	950	$X2$	9.173	1090	$U2$	10.052	995
$Y1$	9.902	1010	BB	10.856	921	Wa	10.671	937	Y	9.515	1051	Ua	10.266	974
$Y2$	10.029	997	BBa	11.065	904	X	10.857	921	Ya	9.633	1038	$V1$	10.457	956
Z	10.273	973	BBb	11.363	880	Xa	11.459	873	$Z1$	9.821	1018	$V2$	10.541	949
Za	10.448	957	CC	11.611	861	Xb	11.914	839	$Z2$	9.921	1008	Va	11.090	902
$AA1$	10.574	946	CCa	12.100	826	Xc	12.271	815	Za	10.102	990	Vb	11.942	837
$AA2$	10.679	936	CCb	12.267	815	Xd	12.453	803	Zb	10.168	983	Vc	12.368	809
AAa	10.876	919	CCc	12.432	804	Xe	12.866	777	AA	10.508	952	Vd	12.493	800
BB	11.089	902	CCd	12.923	774	$Y1$	13.288	753	AAa	10.716	933	W	12.850	778
BBa	11.514	869	DD	13.031	767	$Y2$	13.424	745	BB	10.983	910	X	13.108	763
BBb	11.728	853							BBa	11.418	876	Y	13.352	749
BBc	12.146	823							BBb	11.685	856	Z	13.603	735
BBd	12.672	789							CC	12.776	783	AA	13.739	728
BBe	12.875	777							DD	13.517	740			
BBf	12.991	770							EE	13.835	723			
BBg	13.204	757												
CC	13.507	740												
DD	13.919	718												

* Probably due to impurity in sodium chloride prism.

* The spectrum of 2,2,3,3-tetramethylbutane is not given for the liquid phase since this isomer has the peculiarity of having melting and boiling points separated by only 5.6°C.

[7] See the following paper, R. A. Oetjen and H. M. Randall, Rev. Mod. Phys. **16**, 265 (1944).

[8] R. A. Oetjen, C. L. Kao, and H. M. Randall, Rev. Sci. Inst. **13**, 515 (1942).



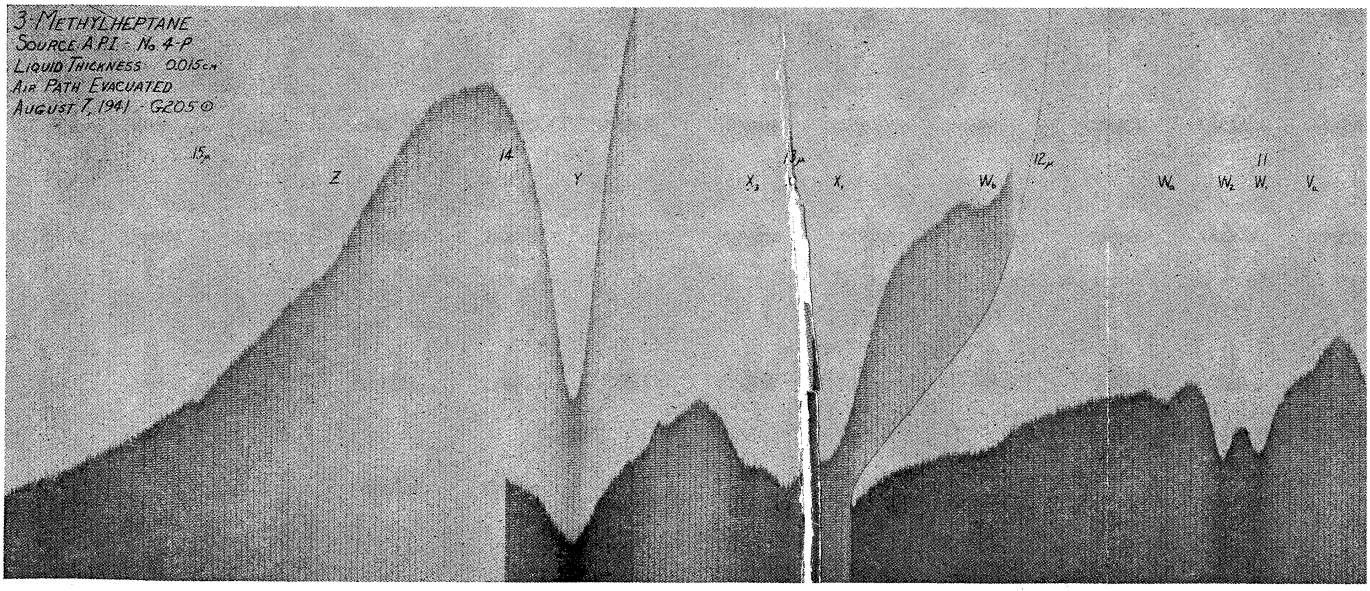
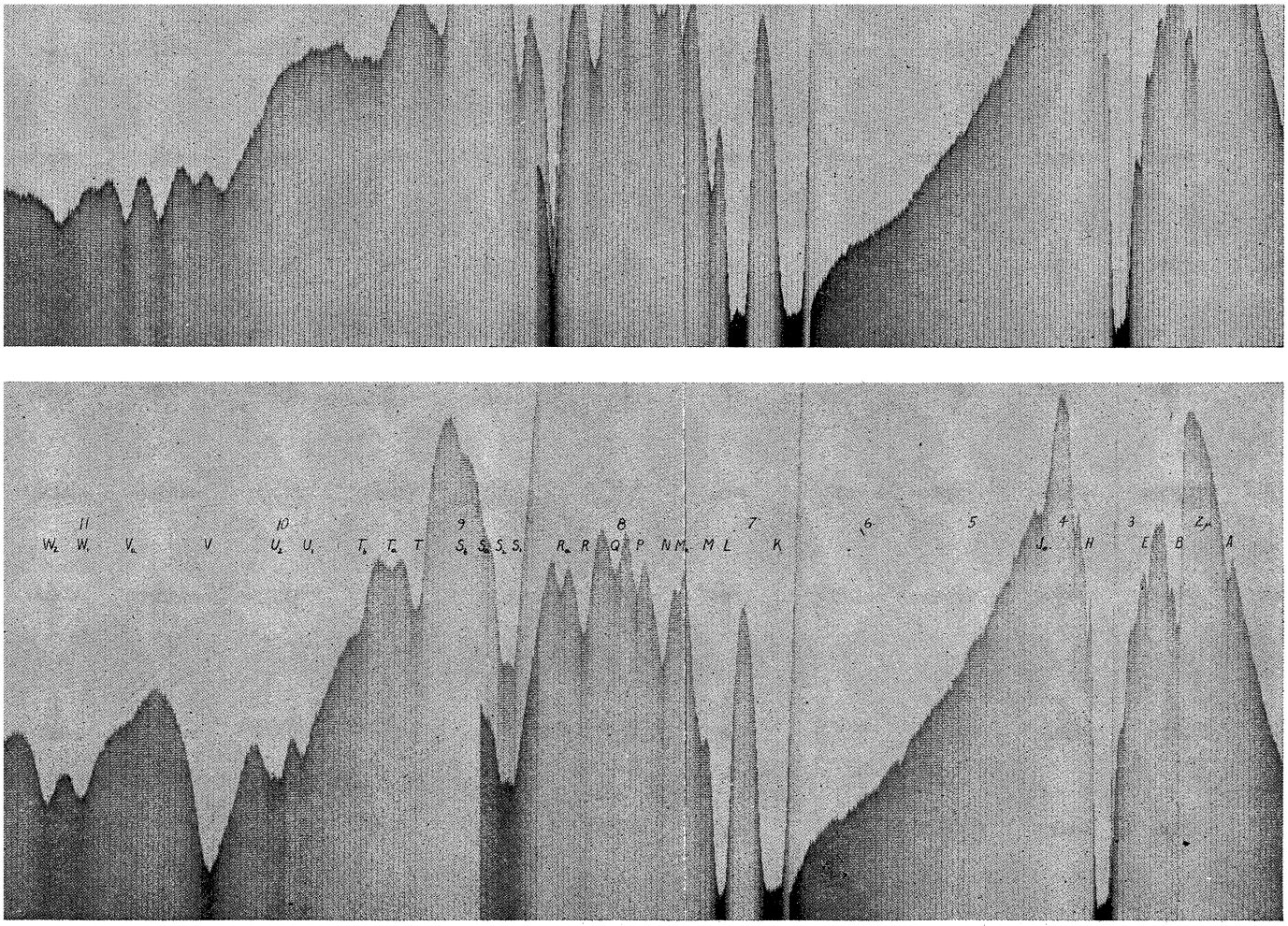


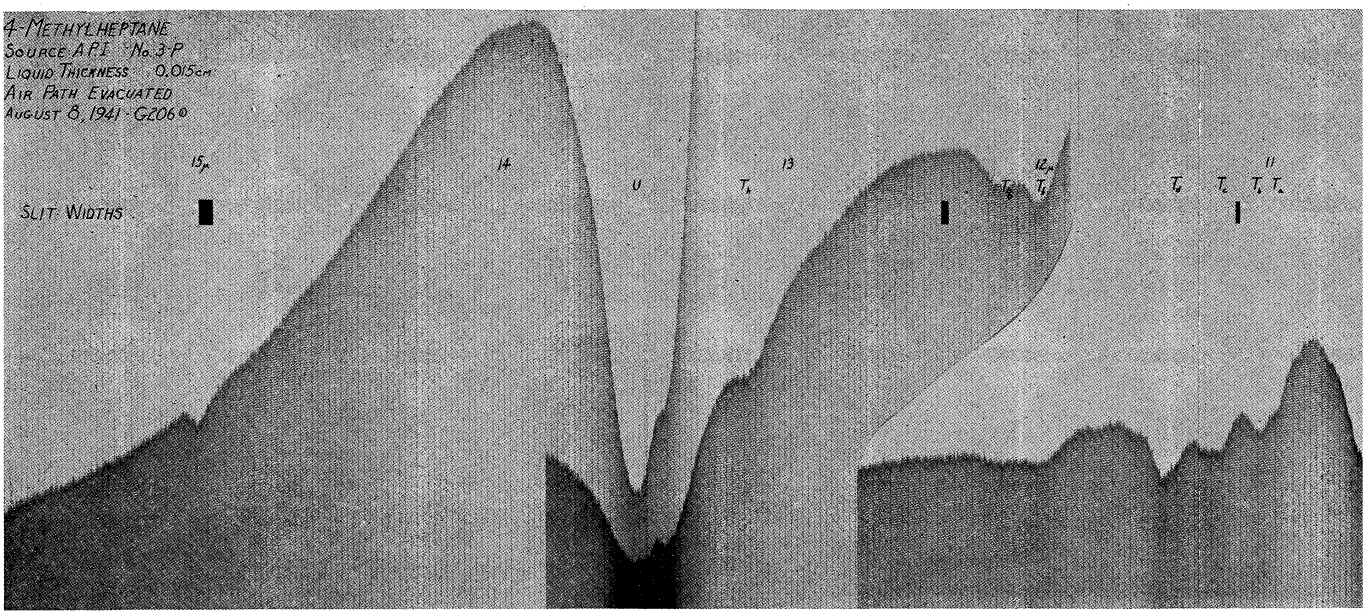
FIG. 1 (top). Infra-red spectrum of *n*-octane.

FIG. 2 (middle). Infra-red spectrum of 2-me



ed spectrum of 2-methylheptane.

FIG. 3 (bottom). Infra-red spectrum of 3-methylheptane.


4-METHYLHEPTANE
SOURCE A.P.I. No. 3-P
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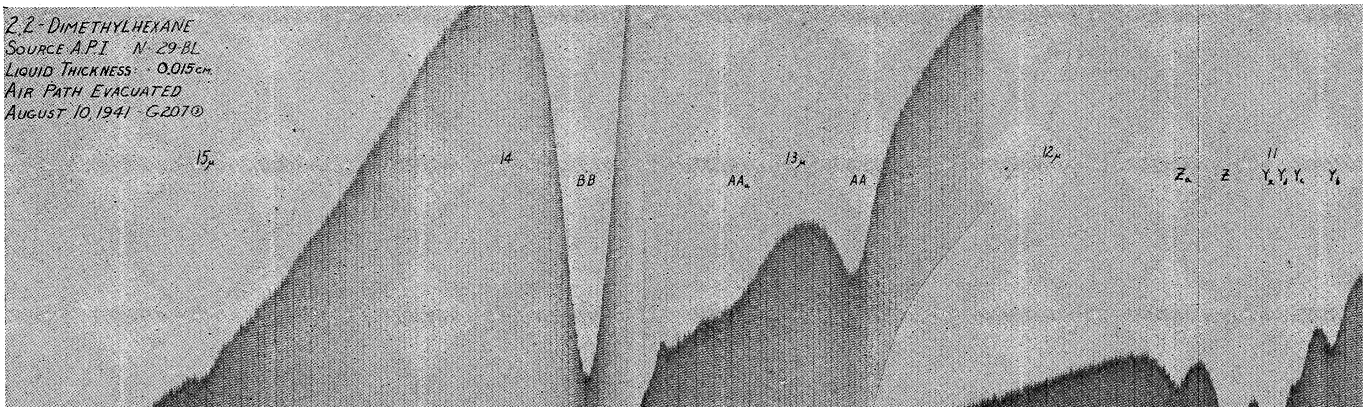
2,2-DIMETHYLHEXANE
SOURCE A.P.I. N-29-BL
LIQUID THICKNESS 0.015cm
AIR PATH EVACUATED
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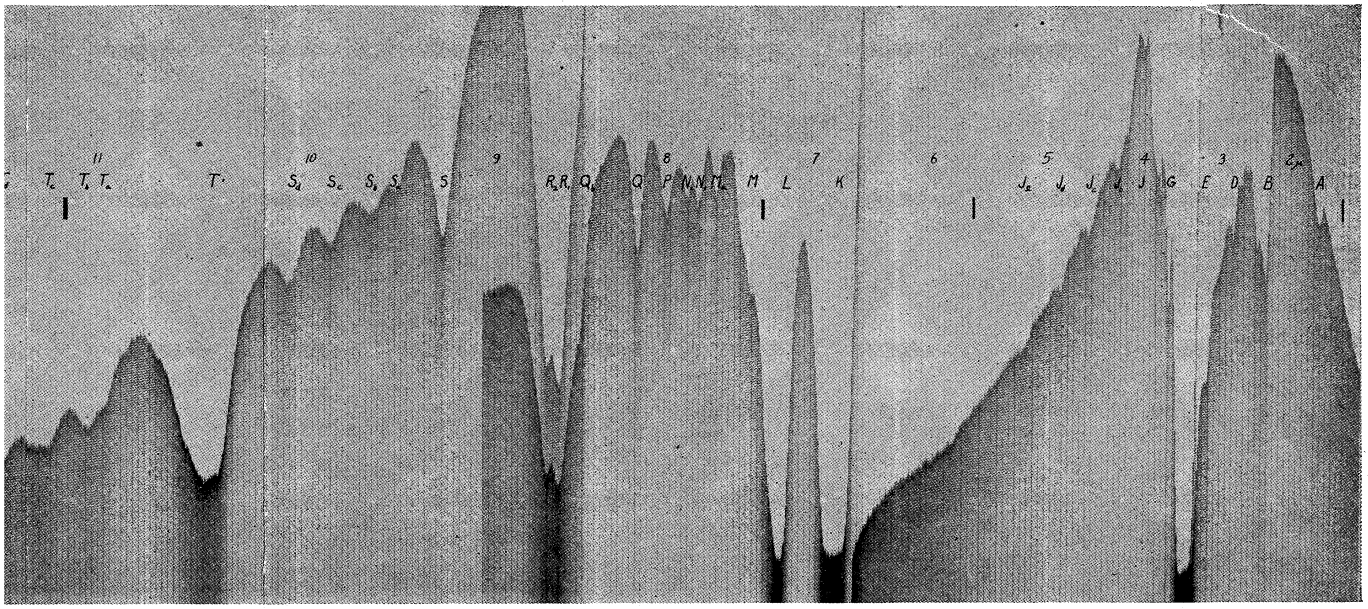
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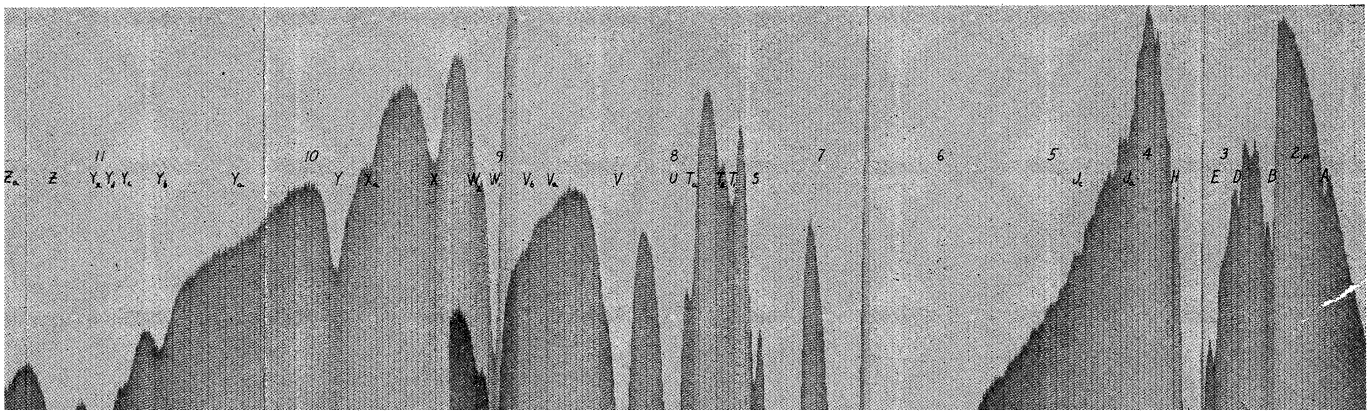
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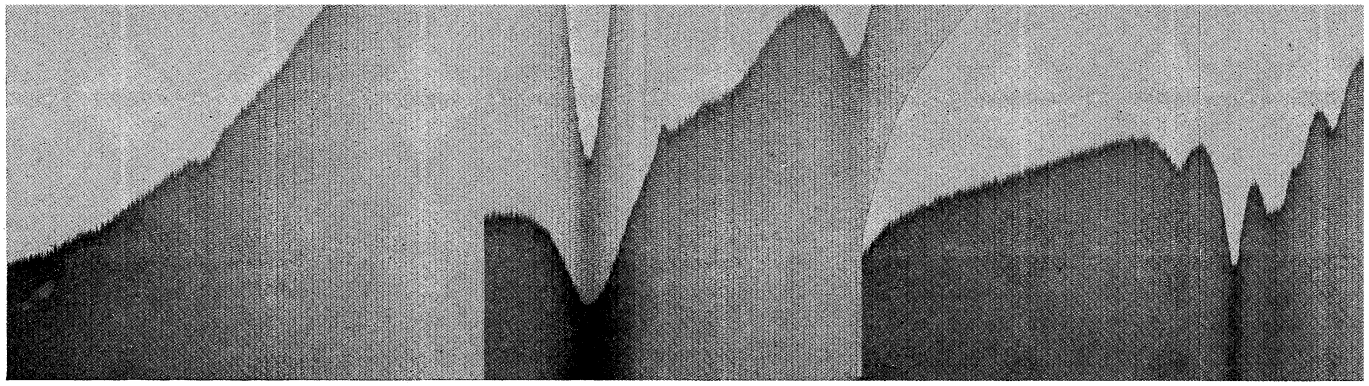
4
3
2
1
Z Z Y Y Y Y Y Y X X W W V V V U T T S J J H E D B A



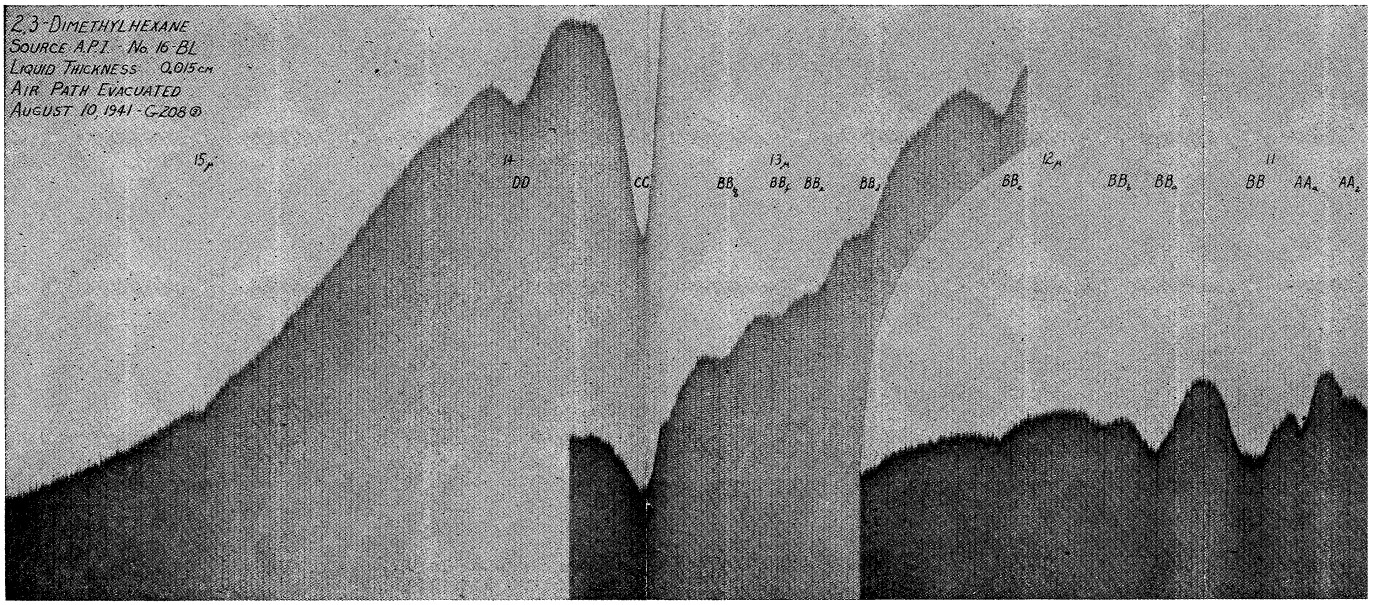
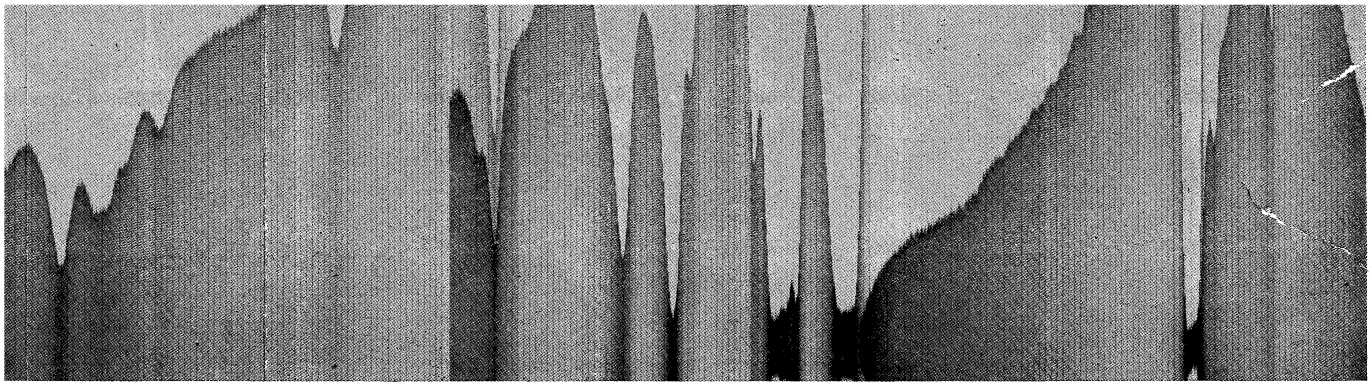
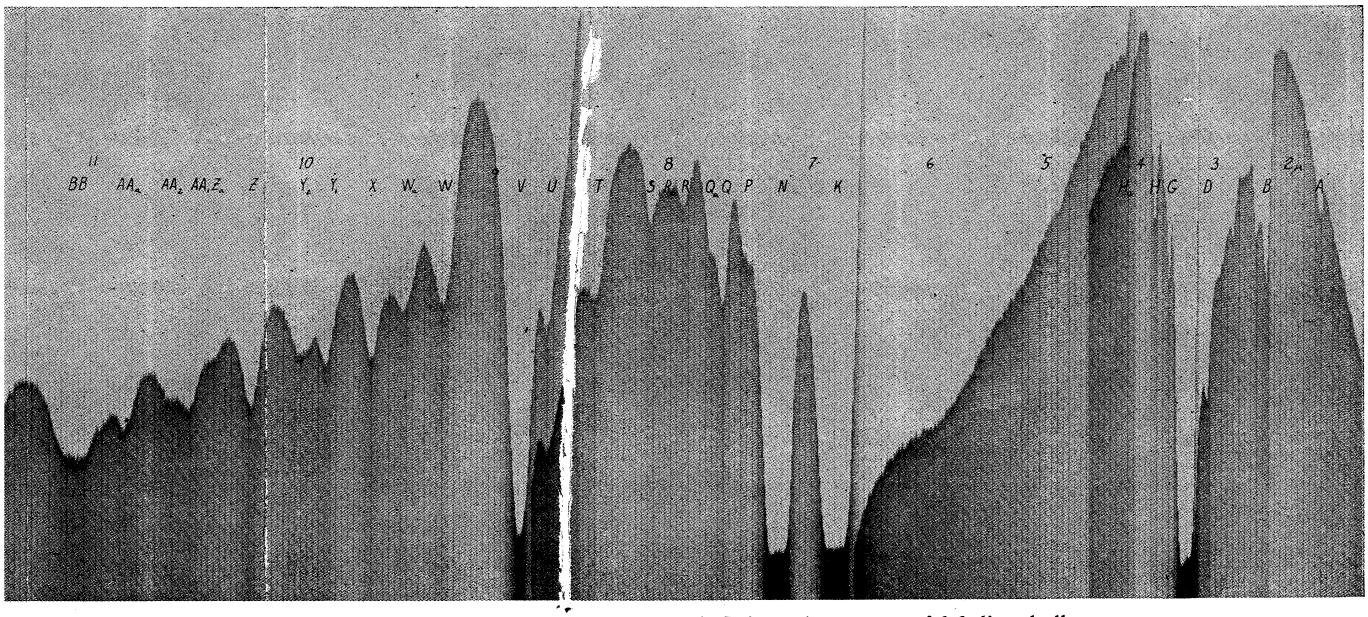


FIG. 4 (top). Infra-red spectrum of 4-methylheptane.

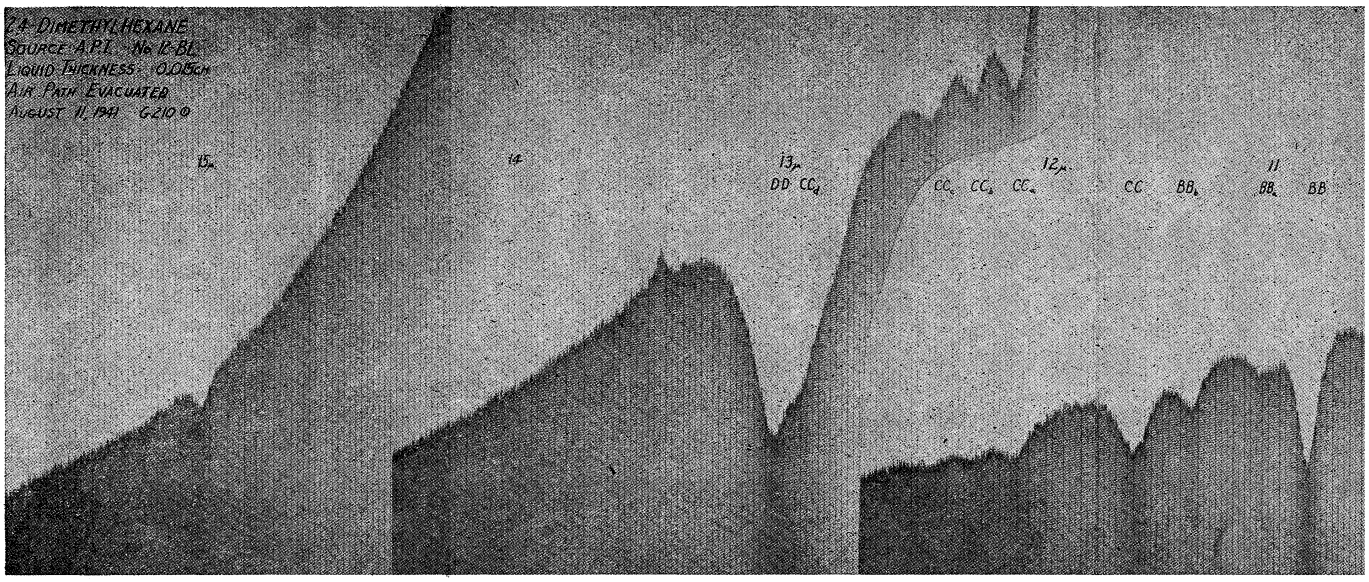
FIG. 5 (middle). Infra-red spectrum of 2,2-

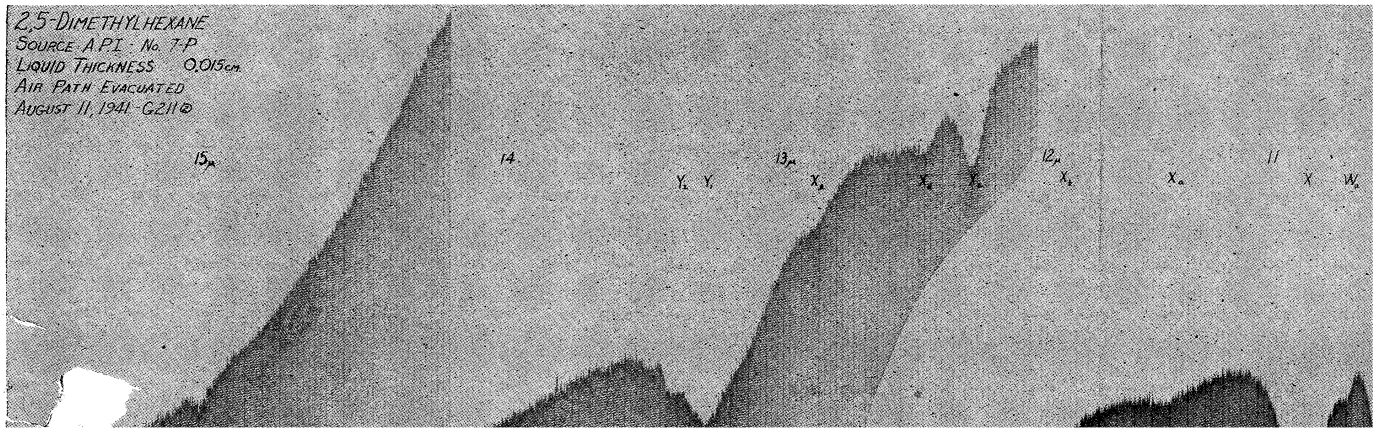


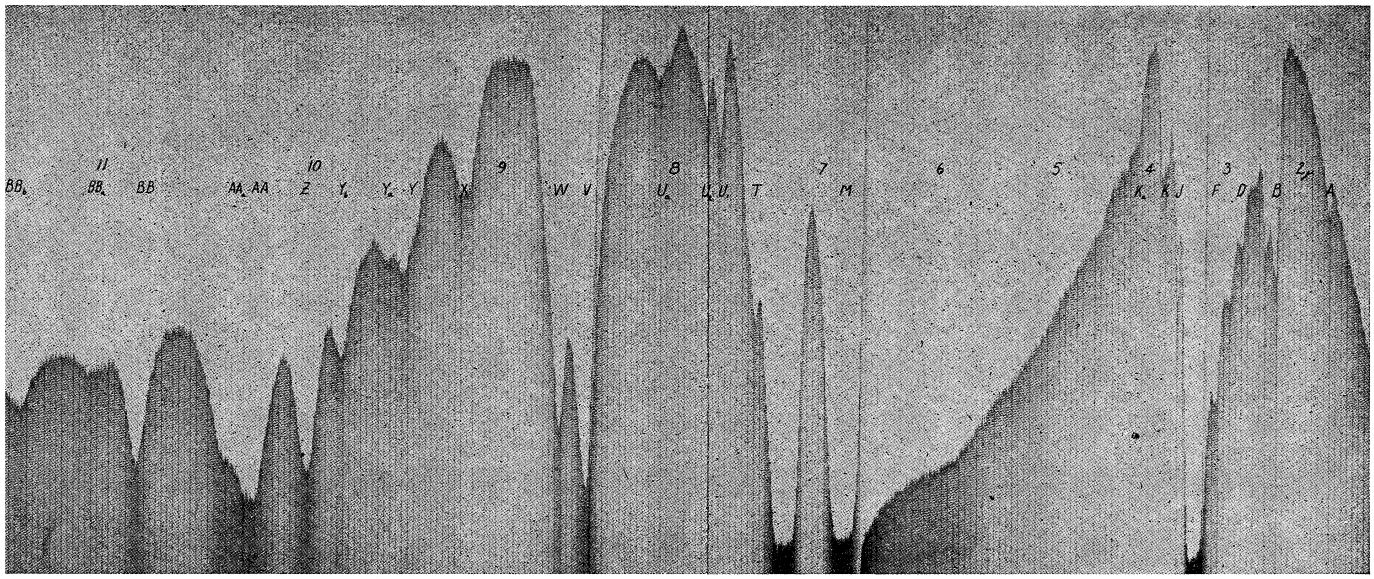


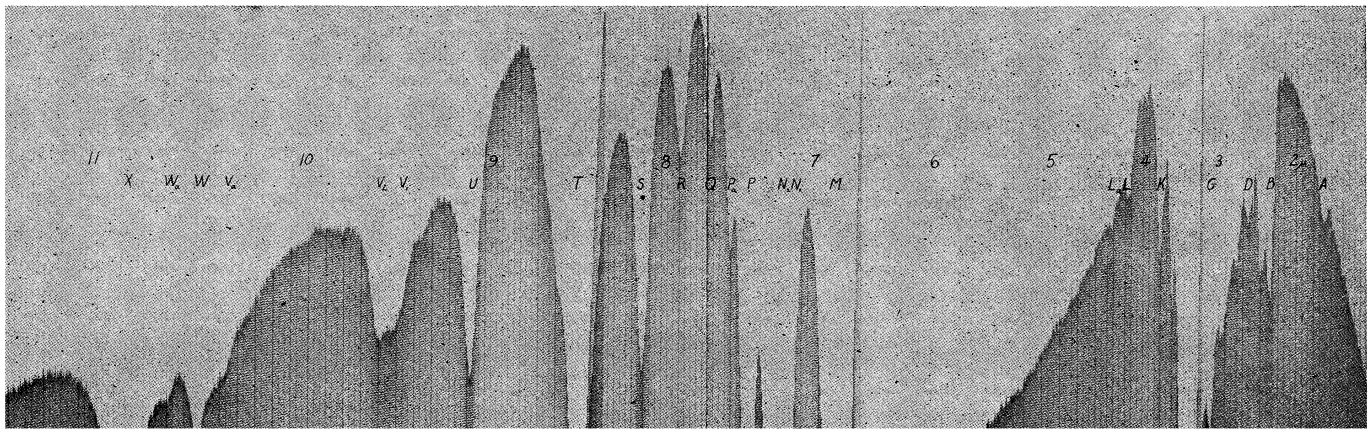
ed spectrum of 2,2-dimethylhexane.

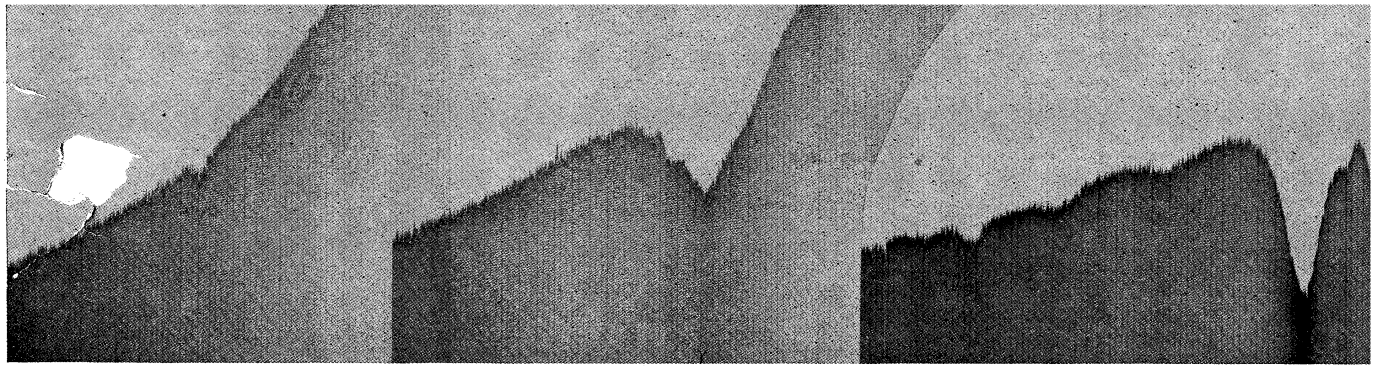
FIG. 6 (bottom). Infra-red spectrum of 2,3-dimethylhexane.


2,4-DIMETHYLHEXANE
SOURCE: A.P.I. No. 12-BL
LIQUID THICKNESS: 0.015cm
AIR PATH EVACUATED
AUGUST 11, 1941 G210
15μ
14
13μ
DD CC4
12μ
CC1 CC2 CC3
CC
BB1
11
BB2
BB


2,5-DIMETHYLHEXANE
SOURCE: A.P.I. No. 7-P
LIQUID THICKNESS 0.015cm
AIR PATH EVACUATED
AUGUST 11, 1941 G211
15μ
14
Y2 Y1
13μ
X3
X4 X5
12μ
X2
X1
11
X
W2


11
BB$_2$
BB$_1$
BB
10
AA$_2$
AA
Z
Y$_3$
Y$_2$
Y
X
9
W
V
8
U$_3$
U$_2$
U$_1$
T
7
M
6
5
4
K$_2$
K$_1$
J
3
F
D
B
2
A


11
X
W$_2$
W
V$_2$
10
V$_1$
V
9
U
T
8
S
R
Q
P
7
N$_2$
N$_1$
M
6
5
4
L$_2$
L$_1$
K
3
G
D
B
2
A



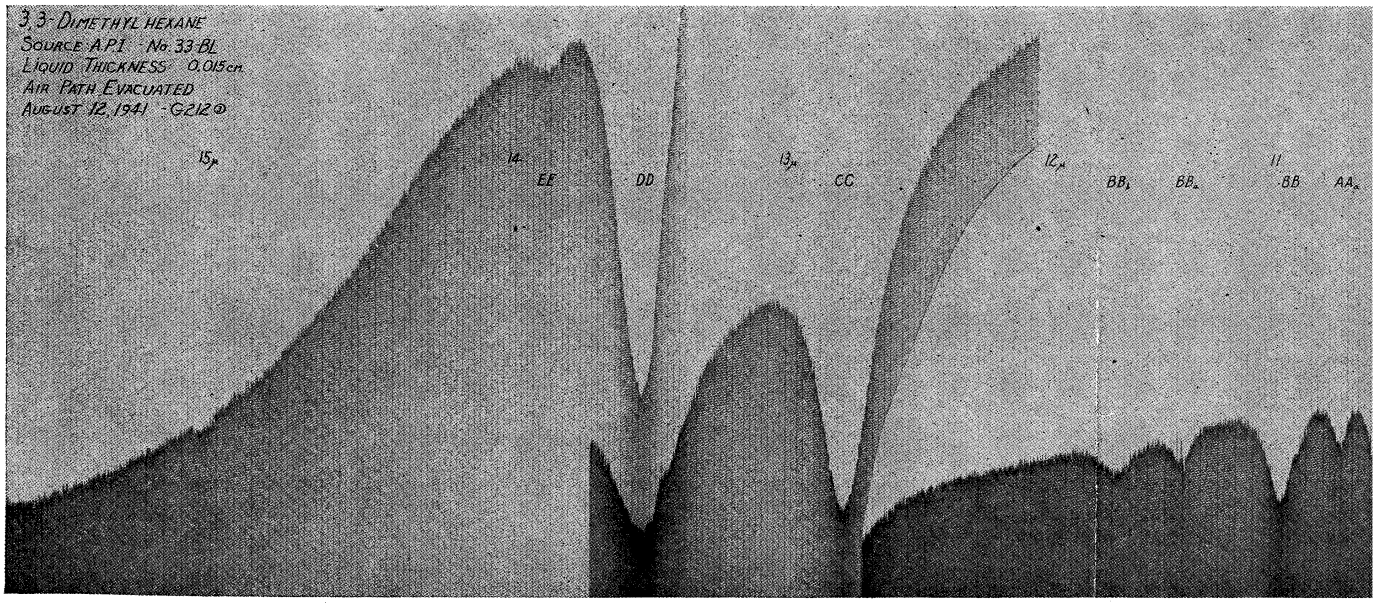
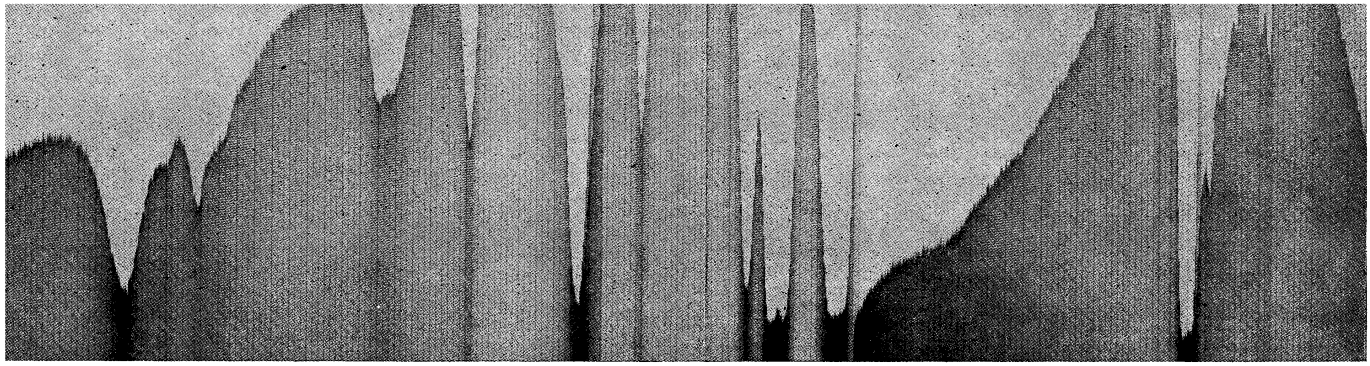
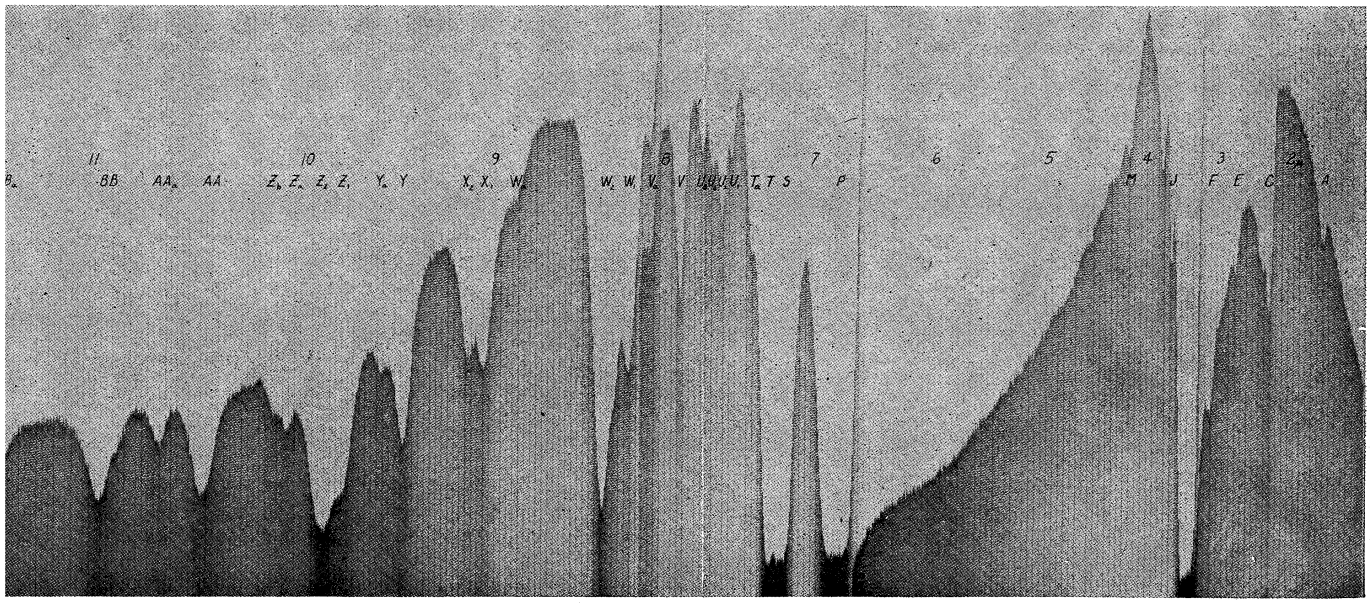


FIG. 7 (top). Infra-red spectrum of 2,4-dimethylhexane.

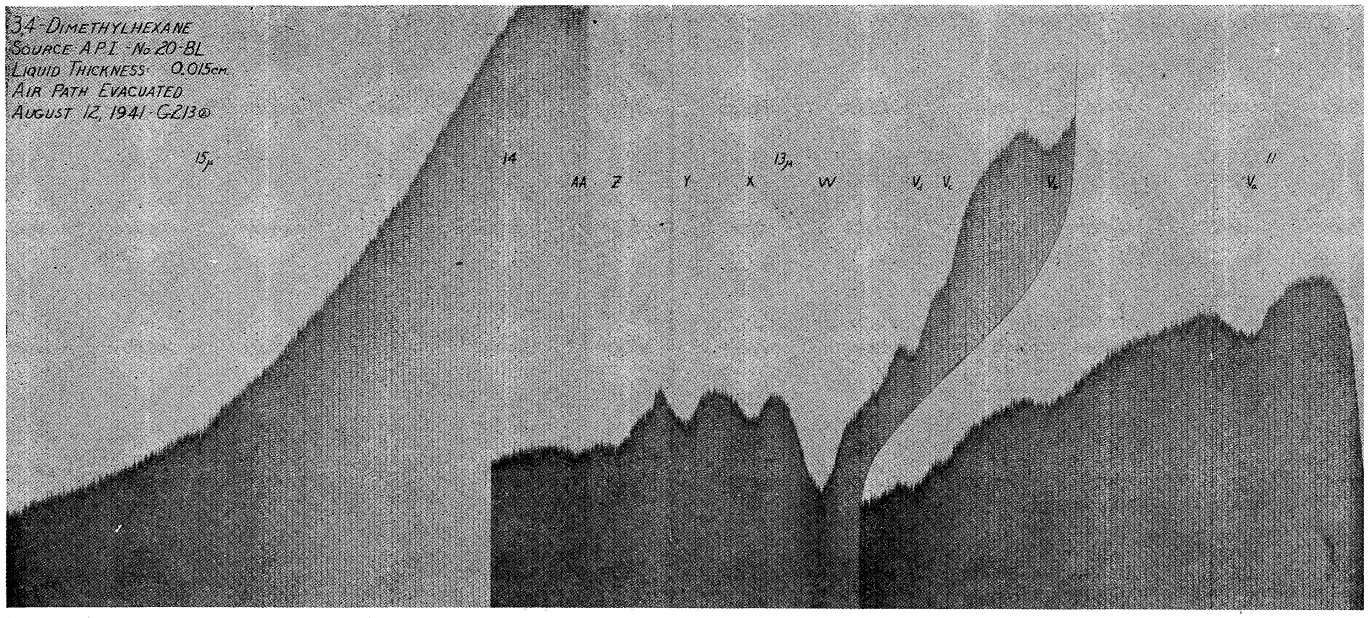
FIG. 8 (middle). Infra-red spectrum of 2,

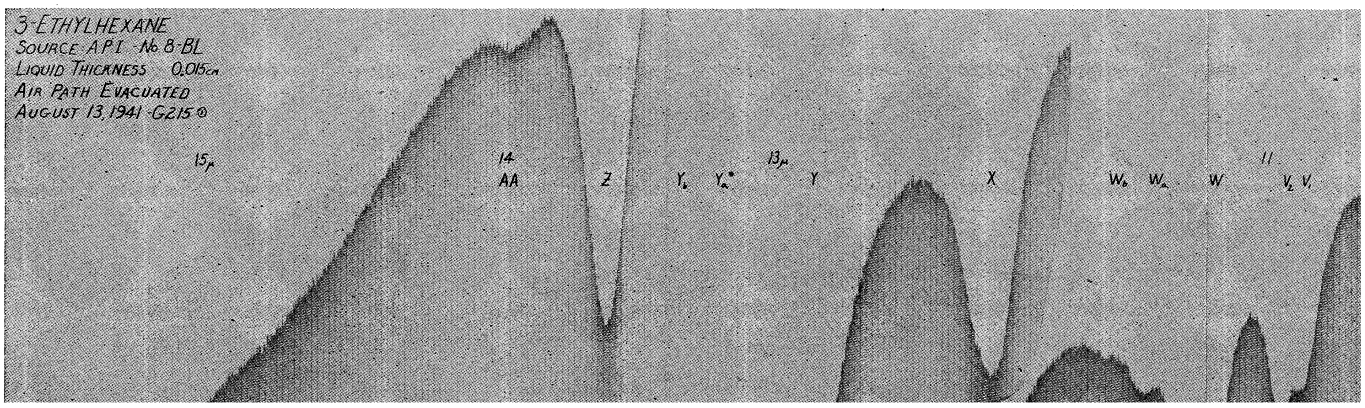


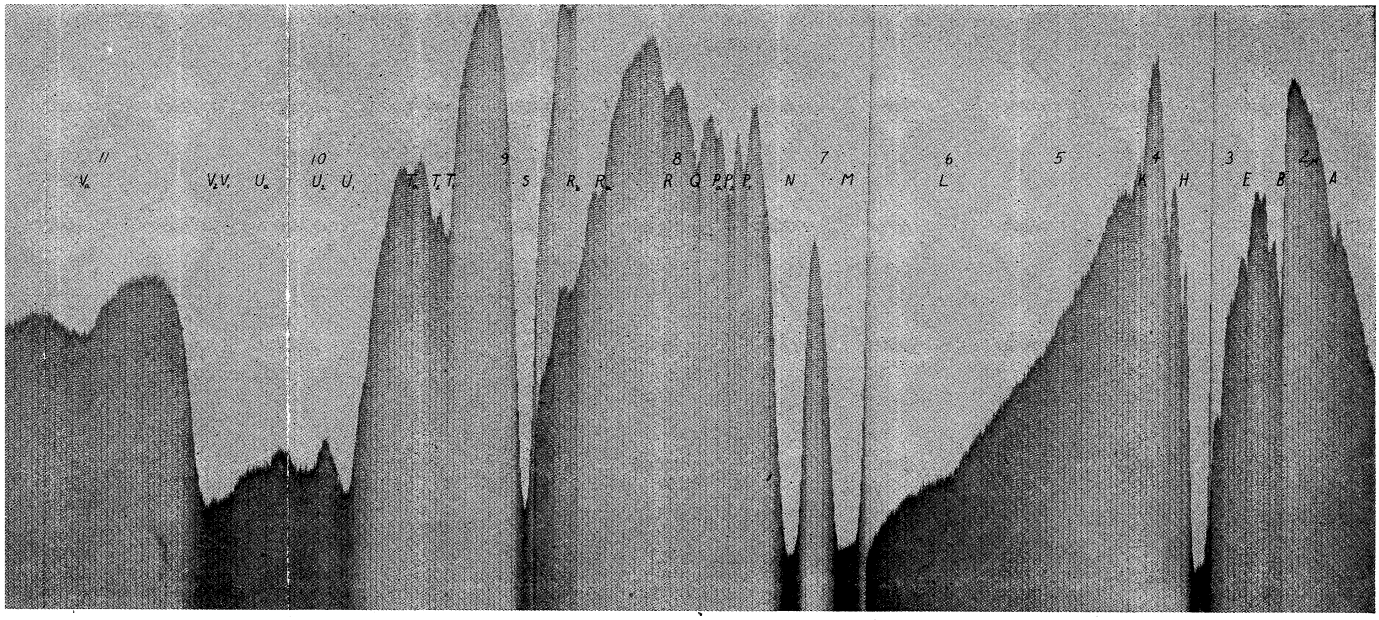


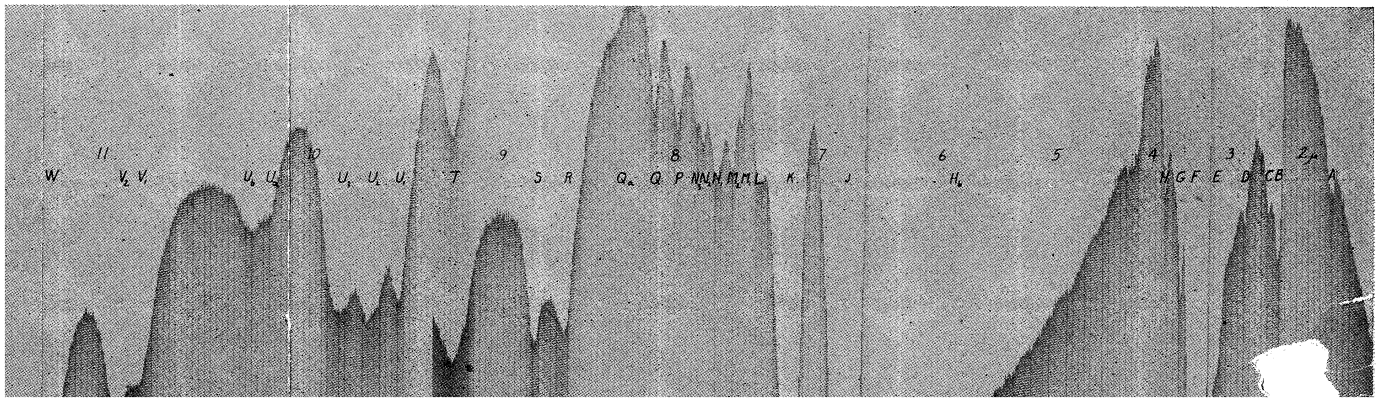
·red spectrum of 2,5-dimethylhexane.

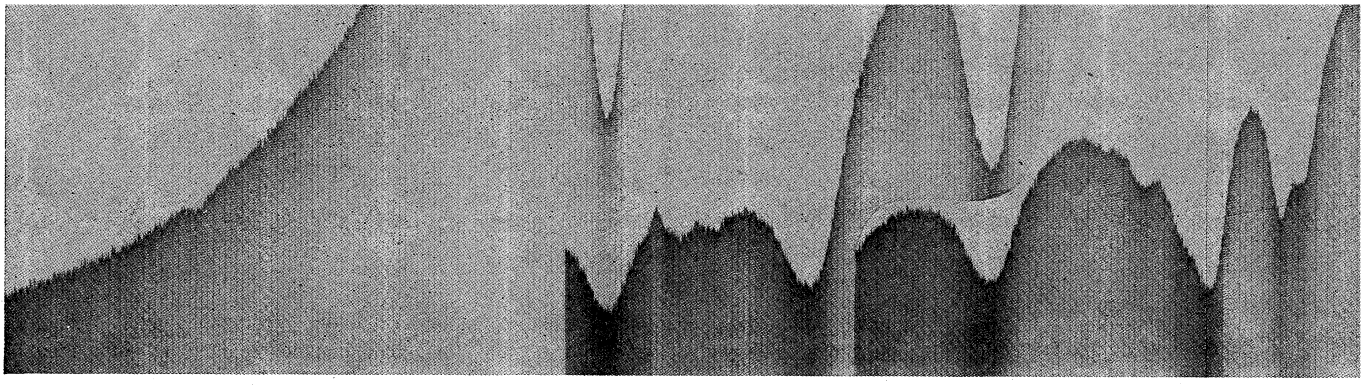
FIG. 9 (bottom). Infra-red spectrum of 3,3-dimethylhexane.


3,4-DIMETHYLHEXANE
SOURCE A.P.I. - No. 20-BL
LIQUID THICKNESS 0.015cm.
AIR PATH EVACUATED
AUGUST 12, 1941 - G213 ®
15μ
14
AA
Z
Y
X
W
13μ
11


3-ETHYLHEXANE
SOURCE A.P.I. No. 8-BL
LIQUID THICKNESS 0.015cm
AIR PATH EVACUATED
AUGUST 13, 1941 - G215 ®
15μ
14
AA
Z
13μ
Y
X
11


11
10
9
8
7
6
5
4
3
2
1
V₂ V₁ V₀ U₂ U₁ T₂ T₁ T₀ S R₂ R₁ R Q P₂ P₁ P N M L K H E B A


11
10
9
8
7
6
5
4
3
2
1
W V₂ V₁ U₂ U₁ U₀ U₁ U₂ T S R Q₂ Q P N₂ N₁ N M₂ M₁ M L K J H₂ M G F E D C B A



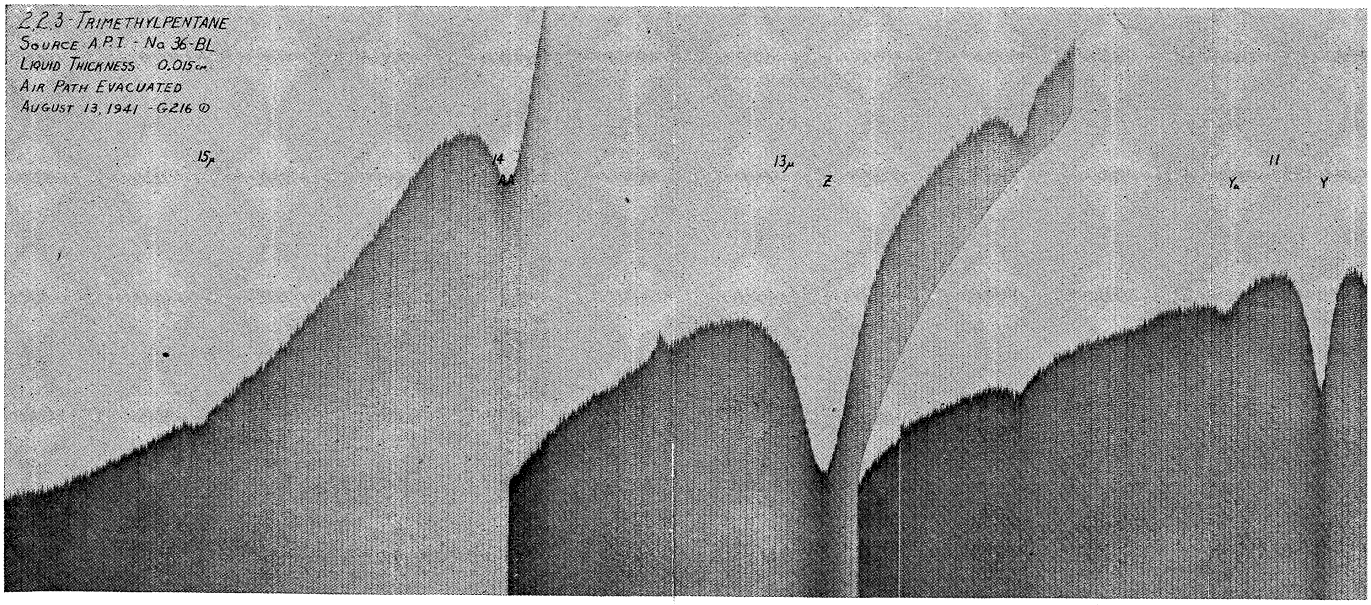
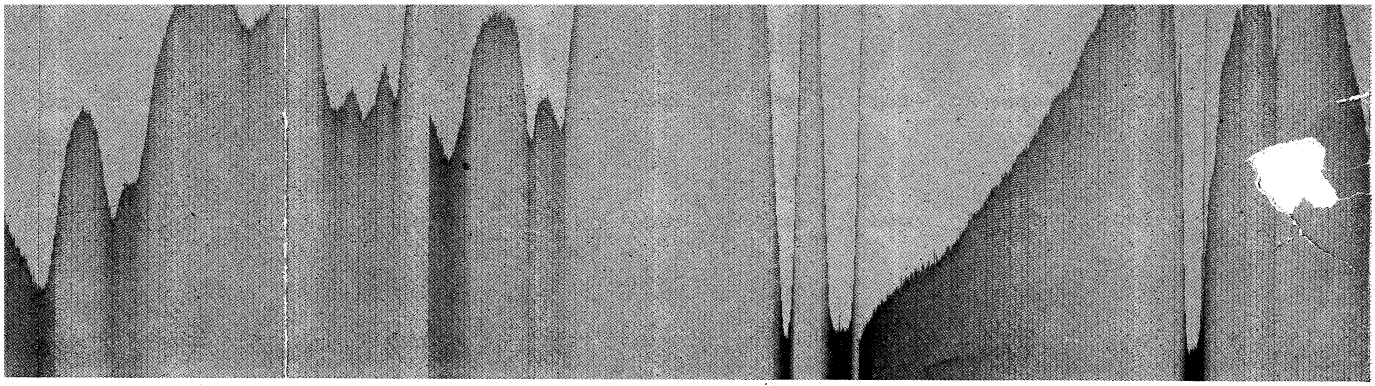
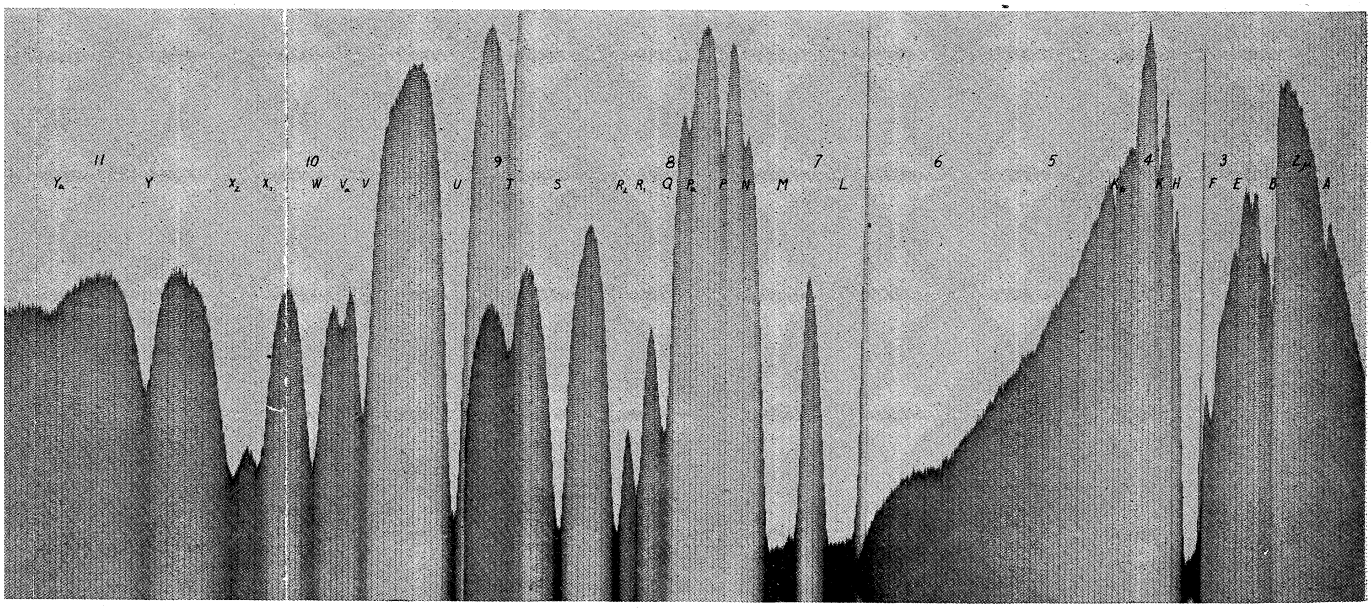


FIG. 10 (top). Infra-red spectrum of 3,4-dimethylhexane.

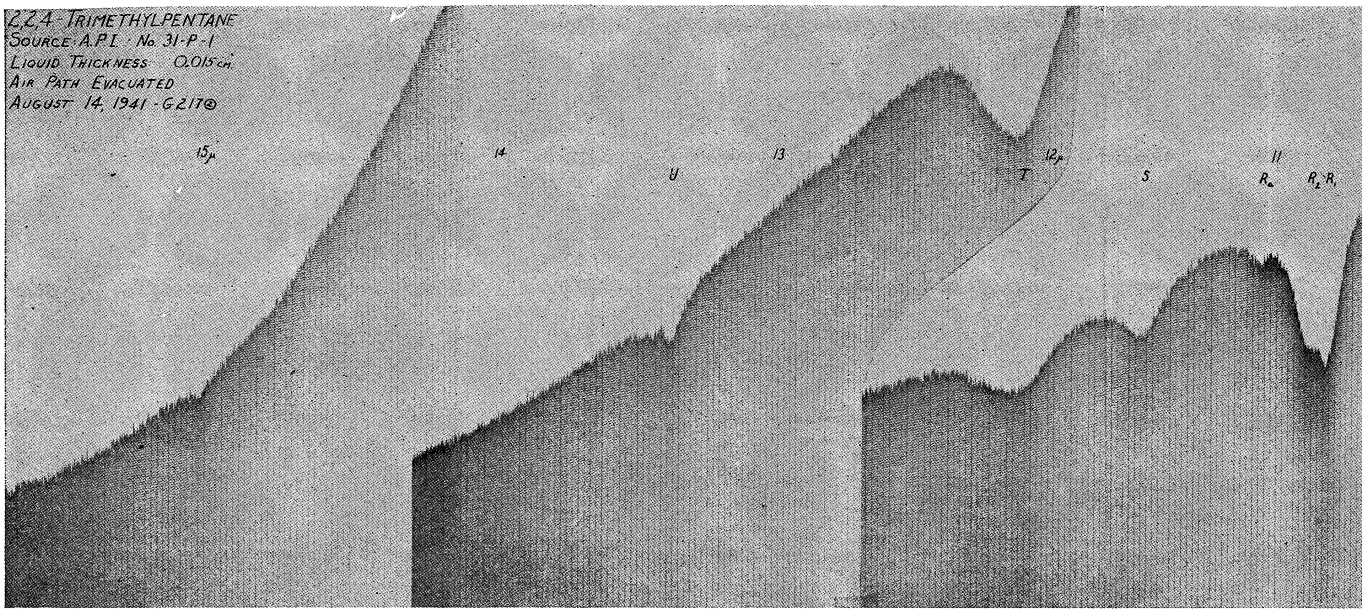
FIG. 11 (middle). Infra-red spectrum of 3

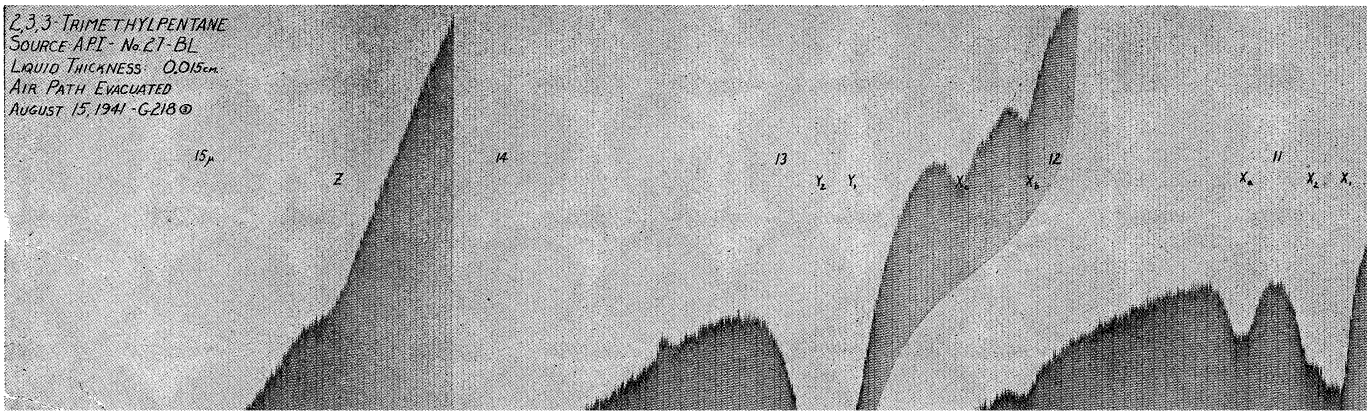


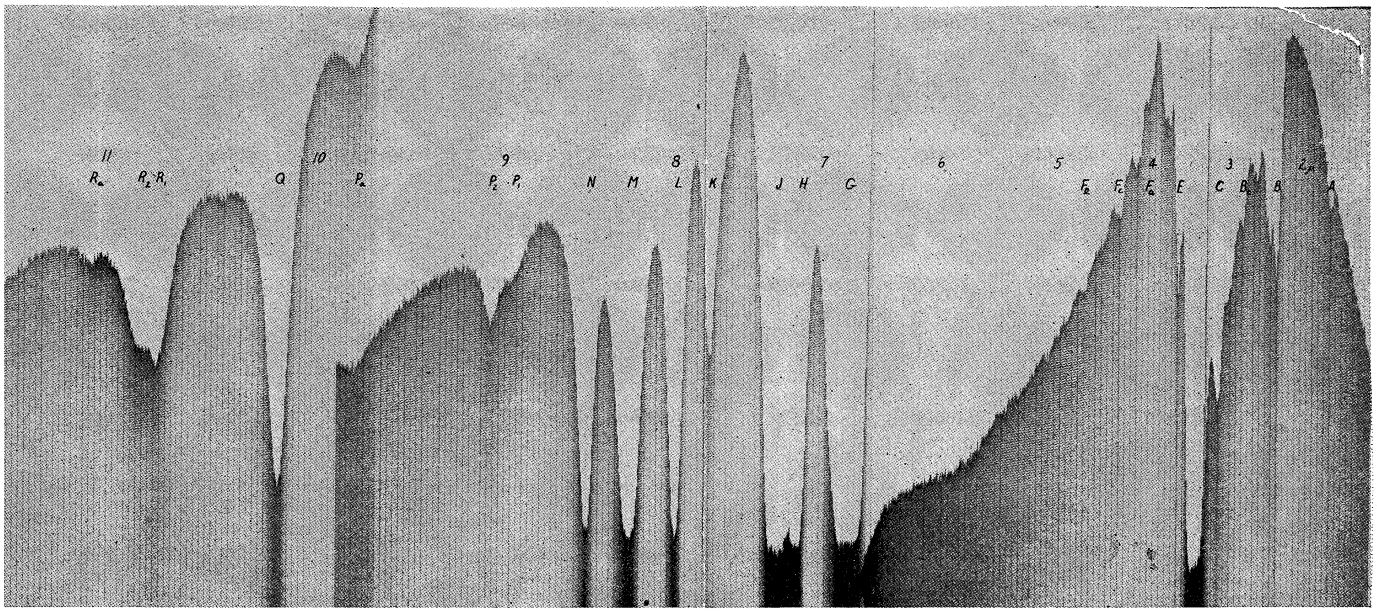


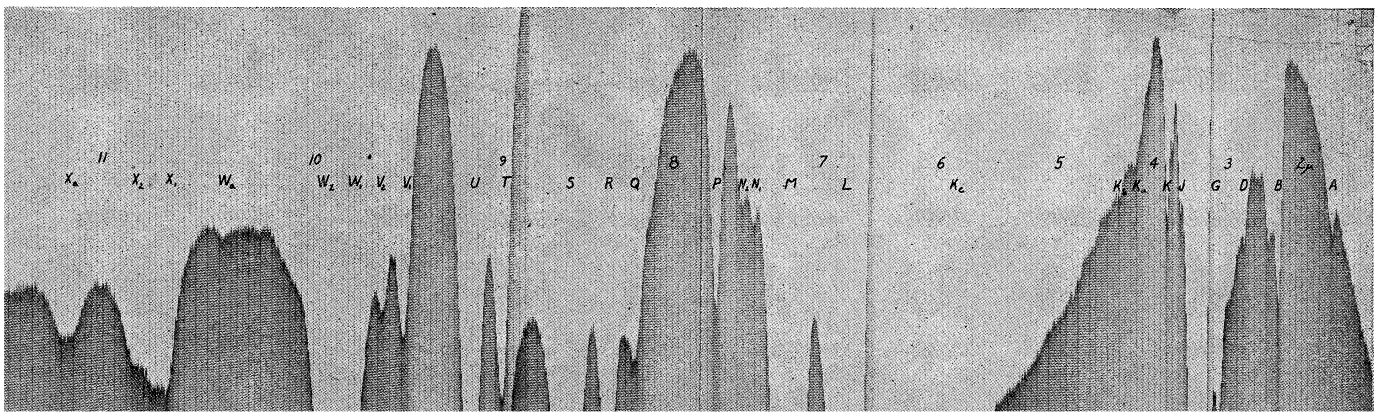
·a-red spectrum of 3-ethylhexane.

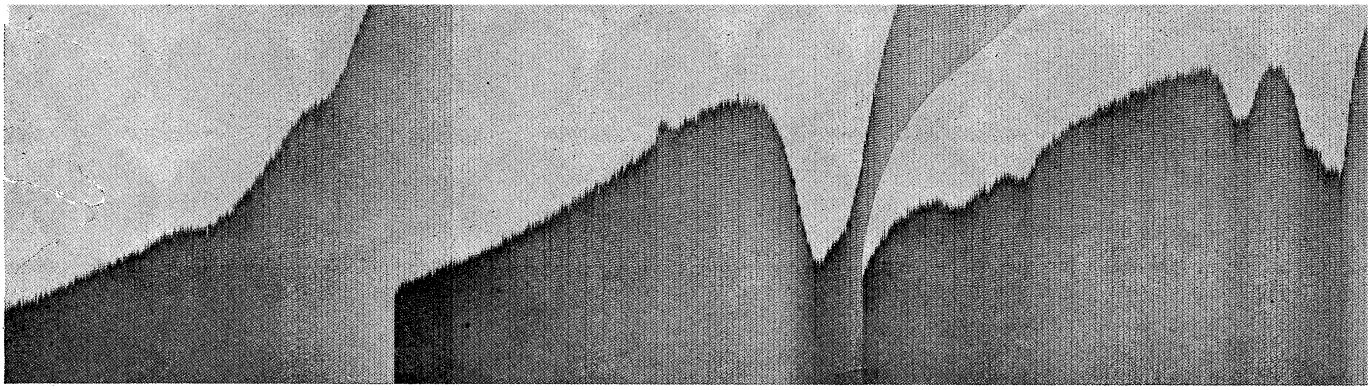
FIG. 12 (bottom). Infra-red spectrum of 2,2,3-trimethylpentane.


2,2,4-TRIMETHYLPENTANE
SOURCE: A.P.I. - No. 31-P-1
LIQUID THICKNESS 0.015 cm.
AIR PATH EVACUATED
AUGUST 14, 1941 - G 217 ⊙
15μ
14
U
13
12μ
T
S
11
R₂
R₁


2,3,3-TRIMETHYLPENTANE
SOURCE: A.P.I. - No. 27-B.L.
LIQUID THICKNESS 0.015 cm.
AIR PATH EVACUATED
AUGUST 15, 1941 - G 218 ⊙
15μ
Z
14
13
Y₂
Y₁
12
X₂
X₁
11
X₂
X₁


11
R_3 R_2 R_1
Q
10
P_3
9
P_2 P_1
N M
8
L K
7
J H C
6
5
E_2 E_1 E_0 E
4
3
C D_1 B
2_{yp}
A


11
X_3 X_2 X_1 W_3
10
W_2 W_1 V_2 V_1
9
U T
S R Q
8
P M_2 M_1 M
7
L
6
K_2
5
K_1 K_0 K J
4
3
G D B
2_{yp}
A



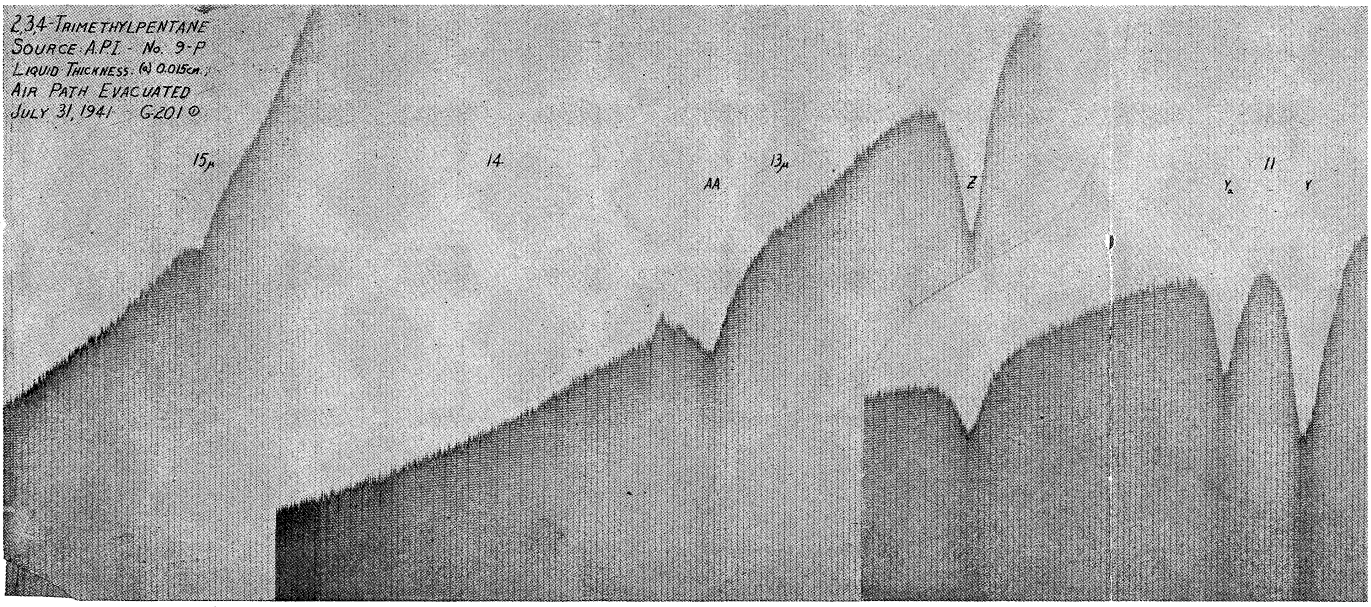
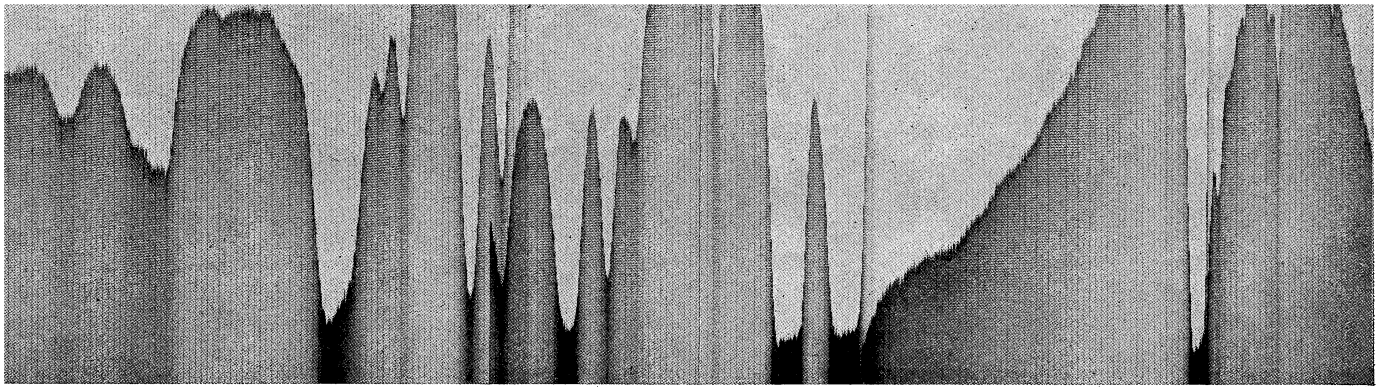
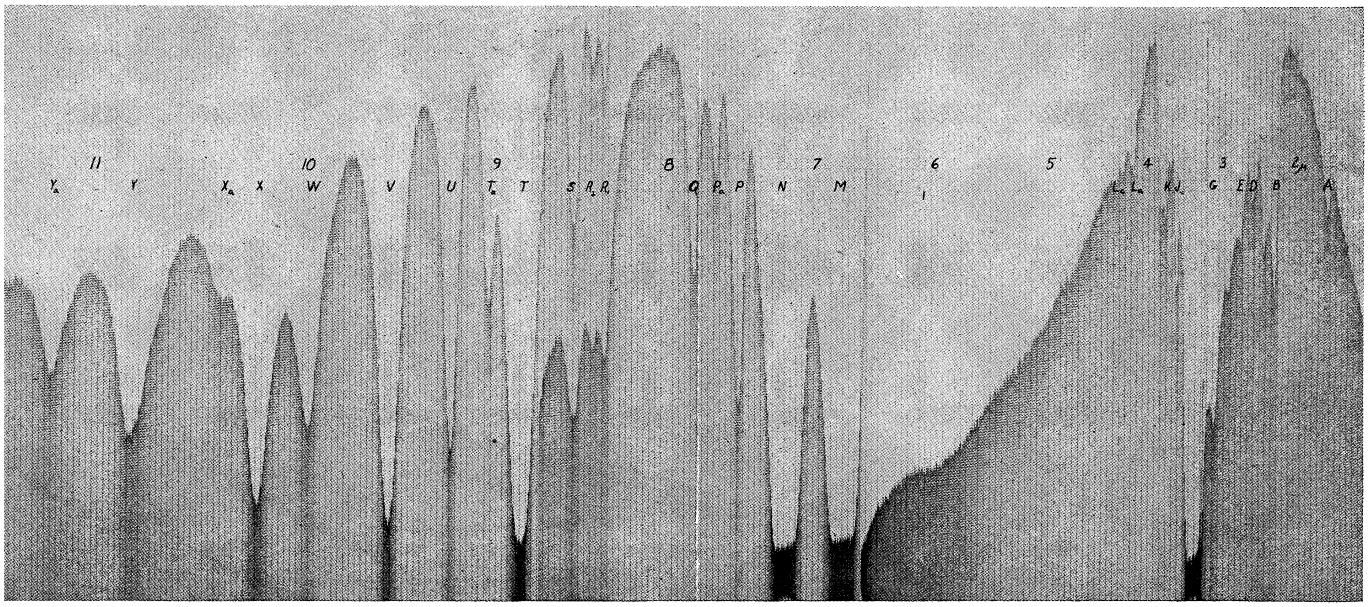


FIG. 13 (top). Infra-red spectrum of 2,2,4-trimethylpentane.

FIG. 14. (middle) Infra-red spectrum of 2,3,





ed spectrum of 2,3,3-trimethylpentane.

FIG. 15 (bottom). Infra-red spectrum of 2,3,4-trimethylpentane.

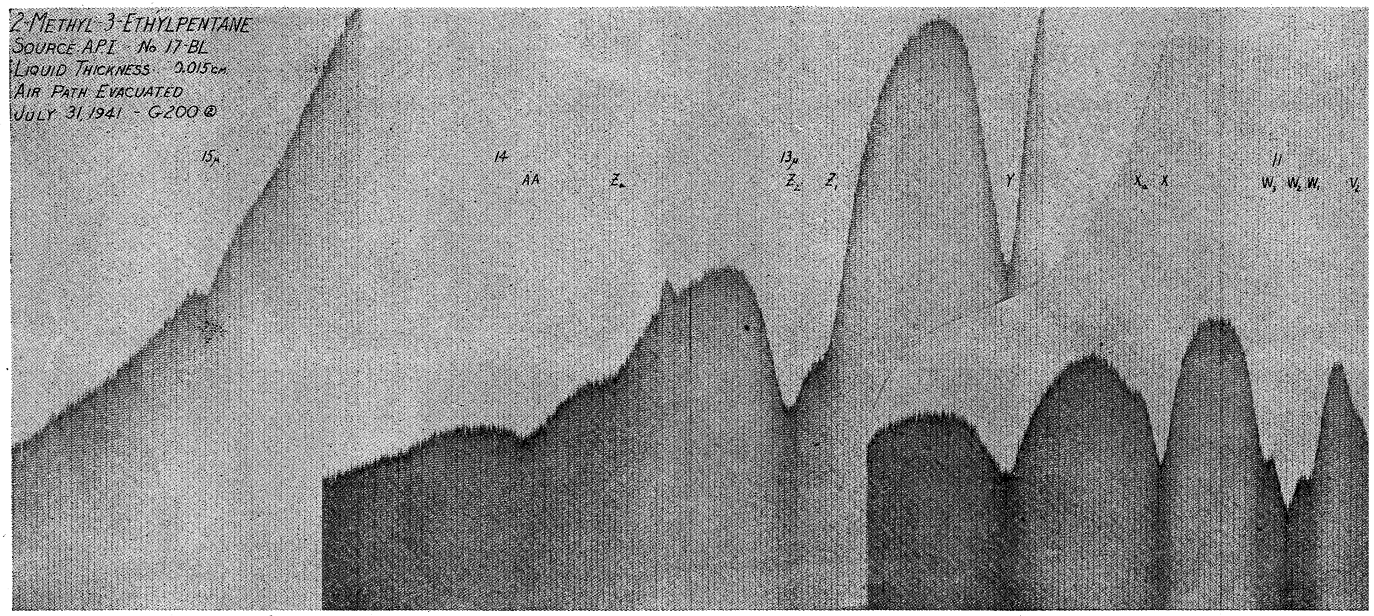


FIG. 16. Infra-red spectrum of 2-meth

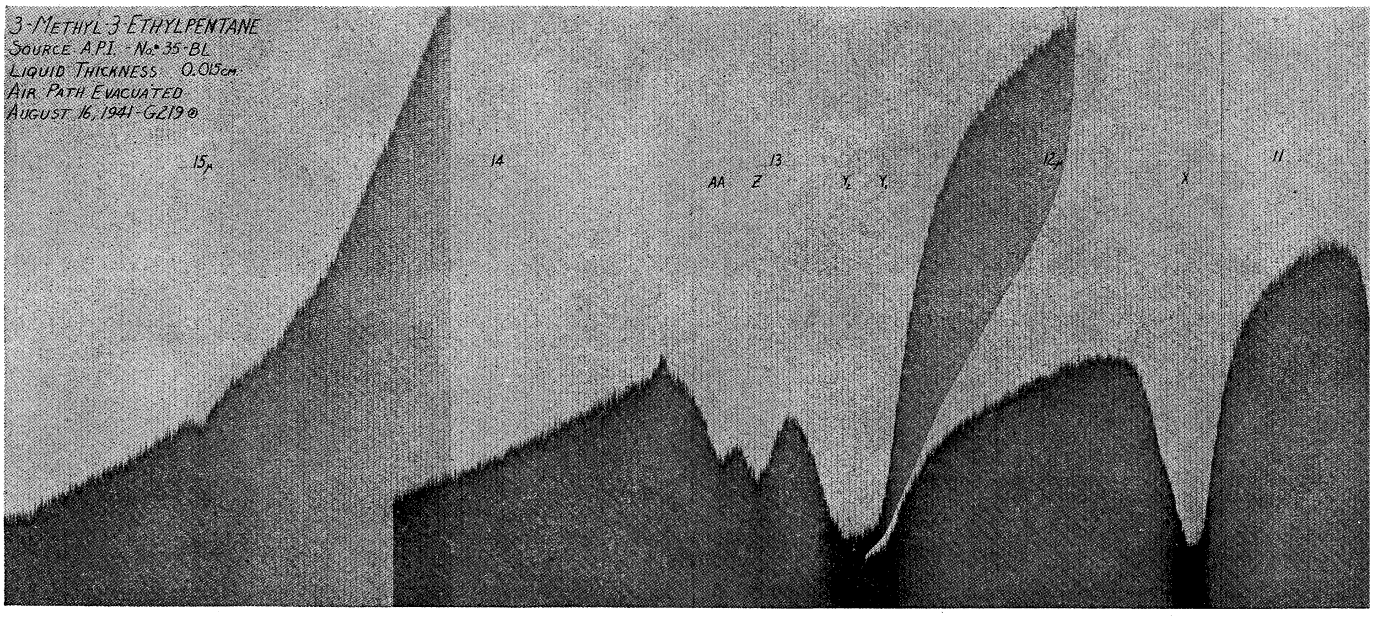
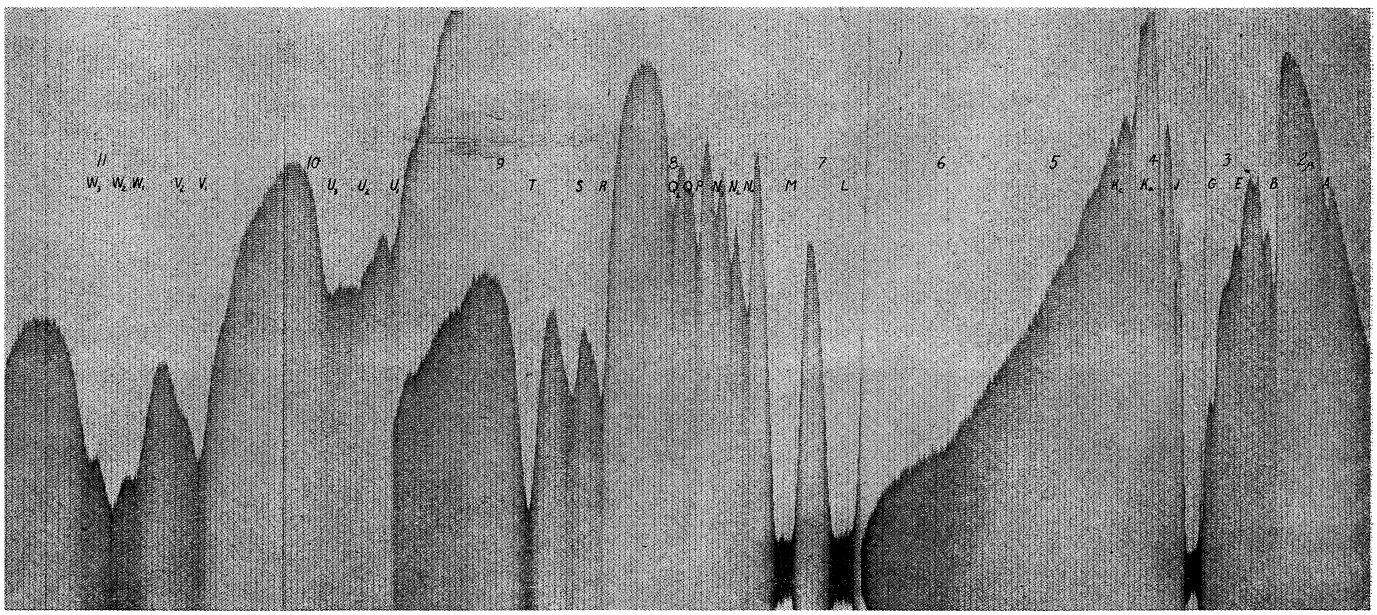
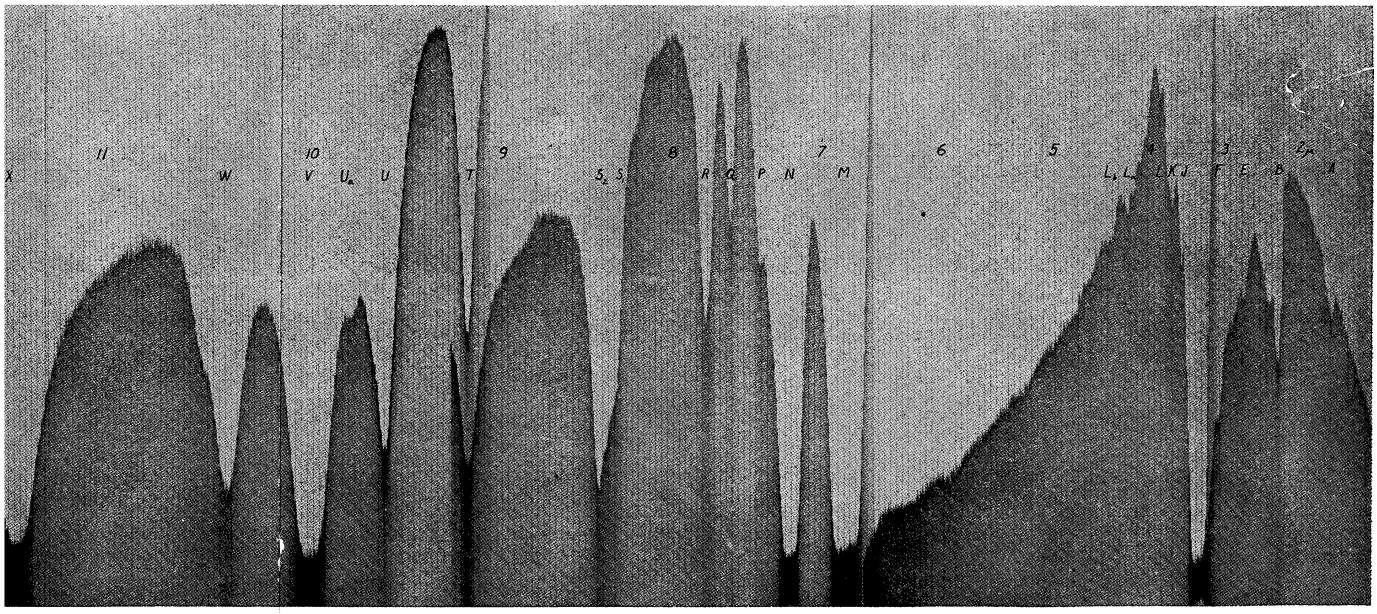


FIG. 17. Infra-red spectrum of 3-meth



spectrum of 2-methyl, 3-ethylpentane.



spectrum of 3-methyl, 3-ethylpentane.

glower operated through a voltage regulator provides the radiation. The detector is a thermopile made by Weyrich. The e.m.f., amplified by the Firestone[9] amplifier, operates a galvanometer, deflections of which are recorded photographically.

The accuracy with which the wave-lengths of absorption lines may be determined depends on several factors including the speed with which the spectrograph is operated, and the sharpness of the line itself. Table II indicates the accuracy with which the wave-length and frequency of a sharp line may be determined with the spectrograph operated as in this investigation.

TABLE III.—*Continued.*

3-Ethylhexane			2,2,3-Trimethylpentane			2,2,4-Trimethylpentane			2,3,3-Trimethylpentane			2,3,4-Trimethylpentane		
Designation	Wave-length (μ)	Wave number (cm^{-1})	Designation	Wave-length (μ)	Wave number (cm^{-1})	Designation	Wave-length (μ)	Wave number (cm^{-1})	Designation	Wave-length (μ)	Wave number (cm^{-1})	Designation	Wave-length (μ)	Wave number (cm^{-1})
A	1.708	5855	*A*	1.686	5931	*A*	1.694	5903	*A*	1.697	5893	*A*	1.700	5882
B	2.316	4318	*B*	2.316	4318	*B*	2.322	4307	*B*	2.314	4322	*B*	2.310	4329
C	2.457	4070	*C*	2.407	4155	B_a	2.408	4153	*C*	2.457	4070	*C*	2.467	4054
*D**	2.769	3611	C_a	2.466	4055	B_b	2.611	3830	*D*	2.606	3837	*D*	2.618	3820
E	3.136	3189	*D*	2.583	3871	B_c*	2.783	3593	*E**	2.783	3593	*E**	2.779	3598
F_1	3.419	2925	*E**	2.777	3601	B_d	2.946	3394	*F*	2.940	3401	*F*	2.960	3378
F_2	3.476	2877	E_a	2.910	3436	*C*	3.140	3185	*G*	3.136	3189	*G*	3.155	3170
G	3.665	2729	*F*	3.142	3183	D_1	3.400	2941	H_1	3.401	2940	H_1	3.402	2939
G_a	3.758	2661	G_1	3.396	2945	D_2	3.478	2875	H_2	3.479	2874	H_2	3.474	2879
H	3.872	2583	G_2	3.479	2874	*E*	3.683	2715	*J*	3.672	2723	*J*	3.672	2723
H_b	6.047	1654	*H*	3.672	2723	F_1	3.813	2623	J_a	3.770	2653	J_a	3.750	2667
J	6.835	1463	*J*	3.805	2628	F_2	3.858	2592	*K*	3.836	2607	*K*	3.819	2618
K	7.243	1381	*K*	3.864	2588	F_a	4.046	2472	K_a	4.207	2377	*L*	3.883	2575
L	7.452	1342	K_a	4.163	2402	F_b	4.185	2389	K_b	4.381	2383	L_a	4.204	2379
M_1	7.564	1322	K_b	4.378	2284	F_c	4.380	2283	K_c	5.971	1675	L_b	4.325	2312
M_2	7.632	1310	*L*	6.806	1469	F_d	4.549	2198	*L*	6.826	1465	L_c	4.389	2278
N_1	7.731	1293	M_1	7.162	1396	F_e	4.752	2104	M_1	7.176	1394	*M*	6.802	1470
N_2	7.821	1279	M_2	7.244	1380	*G*	6.798	1471	M_2	7.242	1381	N_1	7.212	1387
N_3	7.866	1271	M_3	7.316	1367	H_1	7.174	1394	M_3	7.309	1368	N_2	7.263	1377
P	7.993	1251	*N*	7.500	1333	H_2	7.215	1386	N_1	7.482	1337	N_3	7.303	1369
Q	8.142	1228	*P*	7.646	1308	J_1	7.310	1368	N_2	7.553	1324	*P*	7.570	1321
Q_a	8.362	1196	P_a	7.867	1271	J_2	7.382	1355	*P*	7.720	1295	P_a	7.713	1297
R	8.669	1154	*Q*	8.025	1246	*K*	7.778	1286	*Q*	8.248	1212	*Q*	7.860	1272
S	8.849	1130	R_1	8.197	1220	*L*	8.003	1250	*R*	8.414	1188	R_1	8.416	1188
T	9.295	1076	R_2	8.313	1203	*M*	8.290	1206	*S*	8.631	1159	R_2	8.485	1179
U_1	9.583	1044	*S*	8.659	1155	*N*	8.544	1170	*T*	9.022	1108	*S*	8.597	1163
U_2	9.751	1026	*T*	8.952	1117	P_1	8.955	1117	*U*	9.195	1088	*T*	8.900	1124
U_3	9.898	1010	*U*	9.250	1081	P_2	9.103	1099	V_1	9.542	1048	T_a	9.089	1100
U_a	10.225	978	*V*	9.728	1028	P_a	9.812	1019	V_2	9.655	1036	*U*	9.291	1076
U_b	10.306	970	V_a	9.841	1016	*Q*	10.194	981	W_1	9.825	1018	*V*	9.614	1040
V_1	10.841	922	*W*	9.983	1002	R_1	10.783	927	W_2	9.930	1007	*W*	10.023	998
V_2	10.946	914	X_1	10.256	975	R_2	10.871	920	W_a	10.440	958	*X*	10.271	974
W	11.263	888	X_2	10.367	965	R_a	11.075	903	X_1	10.716	933	X_a	10.469	955
W_a	11.570	864	*Y*	10.786	927	*S*	11.575	864	X_2	10.869	920	*Y*	10.872	920
W_b	11.715	854	Y_a	11.211	892	*T*	12.093	827	X_a	11.163	896	Y_a	11.224	891
X	12.170	822	Y_b	12.066	829	*U*	13.406	746	X_b	12.064	828	*Z*	12.280	814
Y	12.875	777	*Z*	12.830	779				X_c	12.325	812	*AA*	13.263	754
Y_a	13.232	756	*AA*	13.965	716				Y_1	12.768	783			
Y_b	13.352	749							Y_2	12.867	777			
Z	13.622	734							*Z*	14.551	687			
AA	13.931	718												

2-Methyl, 3-ethylpentane			2-Methyl, 3-ethylpentane			2-Methyl, 3-ethylpentane			3-Methyl, 3-ethylpentane			3-Methyl, 3-ethylpentane		
Designation	Wave-length (μ)	Wave number (cm^{-1})	Designation	Wave-length (μ)	Wave number (cm^{-1})	Designation	Wave-length (μ)	Wave number (cm^{-1})	Designation	Wave-length (μ)	Wave number (cm^{-1})	Designation	Wave-length (μ)	Wave number (cm^{-1})
A	1.699	5886	K_c	4.392	2277	U_1	9.616	1040	*A*	1.702	5875	*P*	7.446	1343
B	2.316	4318	*L*	6.820	1466	U_2	9.780	1022	*B*	2.317	4316	*Q*	7.640	1309
C	2.457	4070	M_1	7.217	1386	U_3	9.926	1007	*C*	2.460	4065	*R*	7.805	1281
D	2.560	3906	M_2	7.303	1369	V_1	10.567	946	*D*	2.560	3906	S_1	8.368	1195
*E**	2.774	3605	N_1	7.510	1332	V_2	10.660	938	*E**	2.779	3598	S_2	8.471	1180
F	2.923	3421	N_2	7.615	1313	W_1	10.860	921	*F*	3.145	3180	*T*	9.218	1085
G	3.152	3173	N_3	7.715	1296	W_2	10.964	912	H_1	3.415	2928	*U*	9.653	1036
H_1	3.408	2934	*P*	7.829	1277	W_3	11.072	903	H_2	3.483	2871	U_a	9.813	1019
H_2	3.478	2875	Q_1	7.894	1267	*X*	11.520	868	*J*	3.658	2734	*V*	10.033	997
J	3.672	2723	Q_2	7.999	1250	X_a	11.645	859	*K*	3.790	2639	*W*	10.424	959
K	3.845	2601	*R*	8.436	1185	*Y*	12.146	824	*L*	3.920	2551	*X*	11.380	879
K_a	4.029	2482	*S*	8.603	1162	Z_1	12.843	779	L_a	4.294	2329	Y_1	12.658	790
K_b	4.232	2363	*T*	8.861	1129	Z_2	12.986	770	L_b	4.472	2236	Y_2	12.781	782
						Z_a	13.625	734	*M*	6.828	1465	*Z*	13.103	763
						AA	13.921	718	*N*	7.239	1381	*AA*	13.242	755

* Probably due to impurity in sodium chloride prism.

[9] F. A. Firestone, Rev. Sci. Inst. **3**, 163 (1932).

The cell for holding the liquid sample is a mercury-sealed cell which has already been described.[10] The cell consists of two sodium chloride plates separated by a flat platinum shim. The thickness of the liquid sample is that of the shim. Channels in the salt plates which surround the sample chamber are filled with mercury, this serving to prevent the sample from escaping when the cell is placed in the evacuated chamber. The sample chamber is filled through holes drilled in the salt plates. These holes are closed by small pieces of synthetic rubber which is unaffected by the octanes. The salt plates are clamped together with two metal plates. Rather thick rubber gaskets are used between the metal and the salt to prevent strain and breakage of the salt plates.

In this investigation different cell thicknesses were used, the data given here being those for a thickness of 0.015 cm.

[10] H. M. Randall, Rev. Sci. Inst. **10**, 195 (1939).

DATA

Figures 1 through 17 are photographs of the spectra as they are recorded.

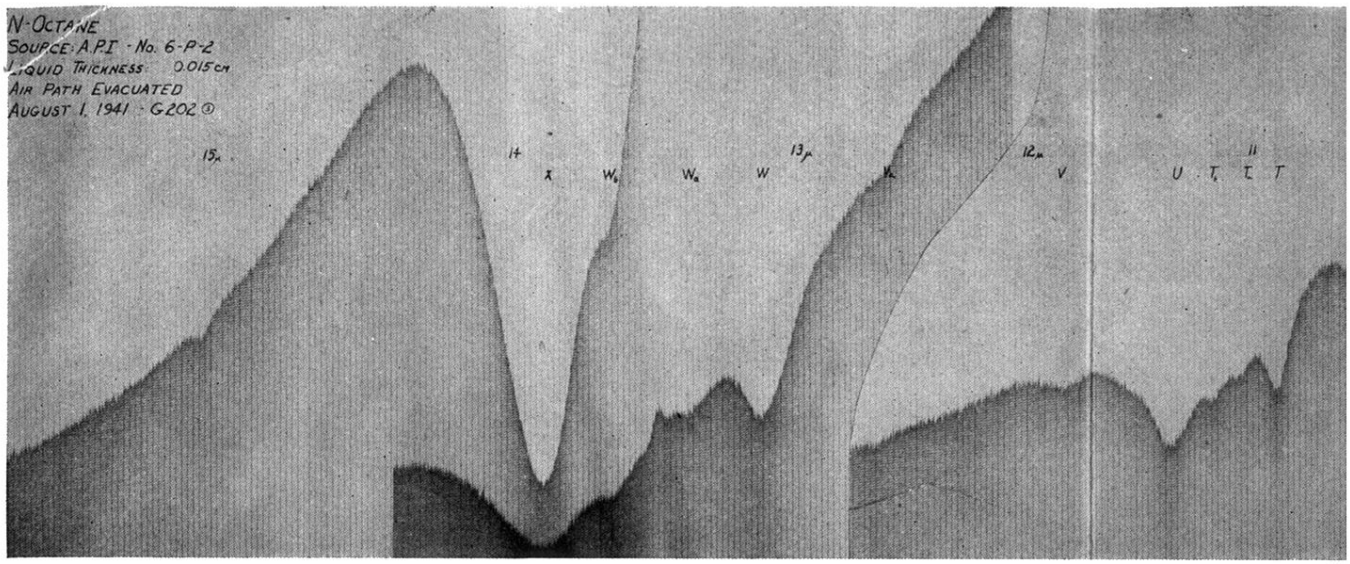
Table III gives the location of each absorption line in terms of wave-length and wave numbers. Similarly designated absorption lines in the spectra of different isomers are unrelated.

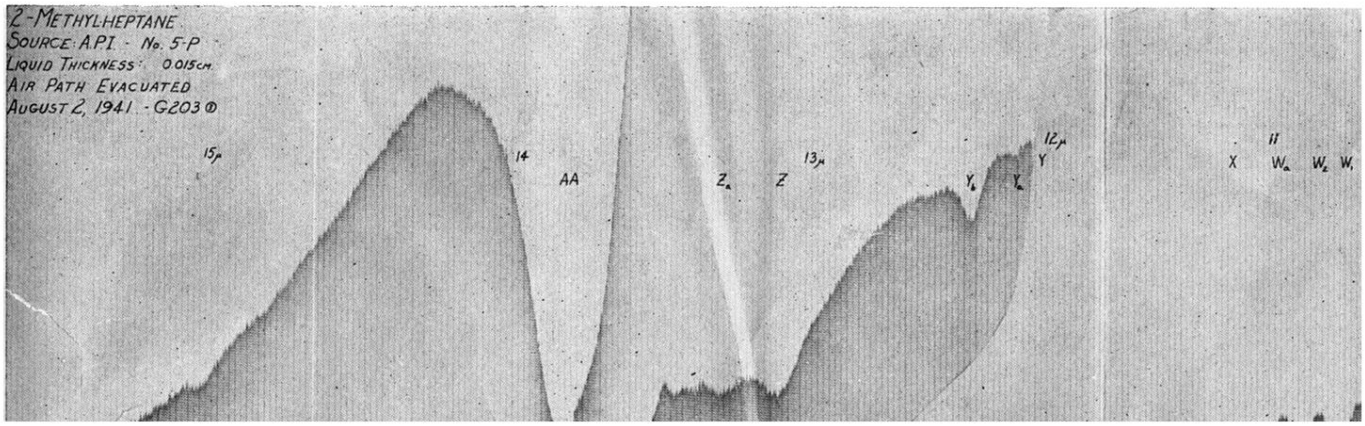
It should be pointed out that the absorption line at 2.78μ or 3600 cm^{-1} which occurs in each of the spectra is due not to the octanes, but rather to some other source which has not yet been satisfactorily explained.

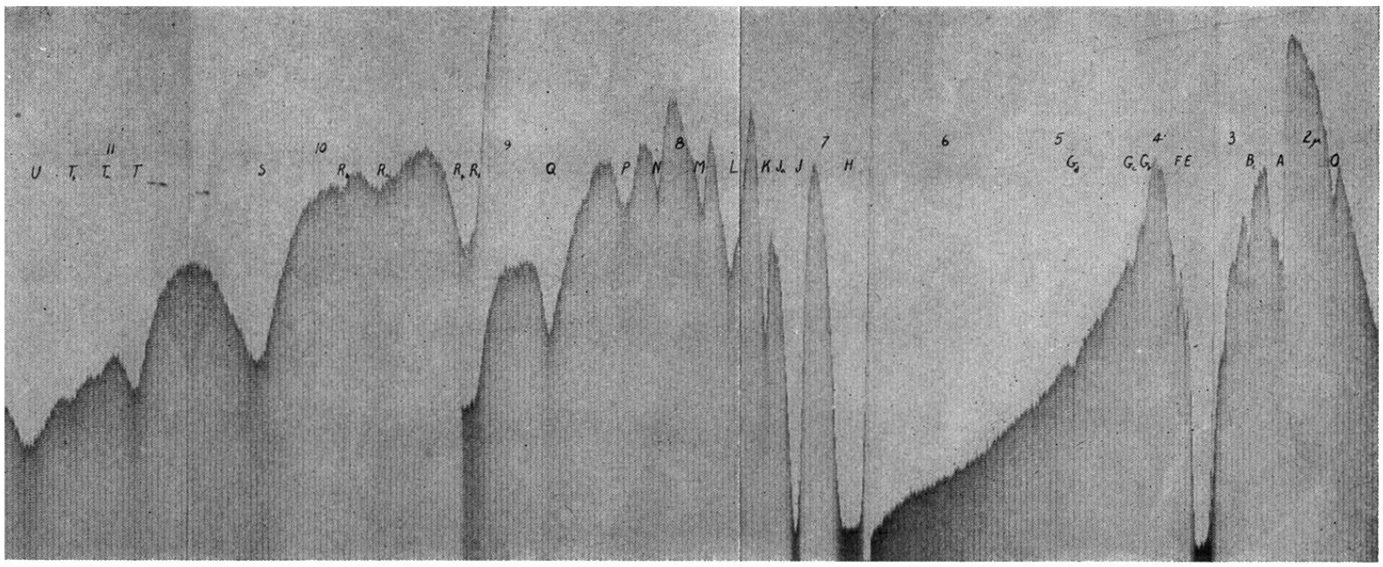
ACKNOWLEDGMENTS

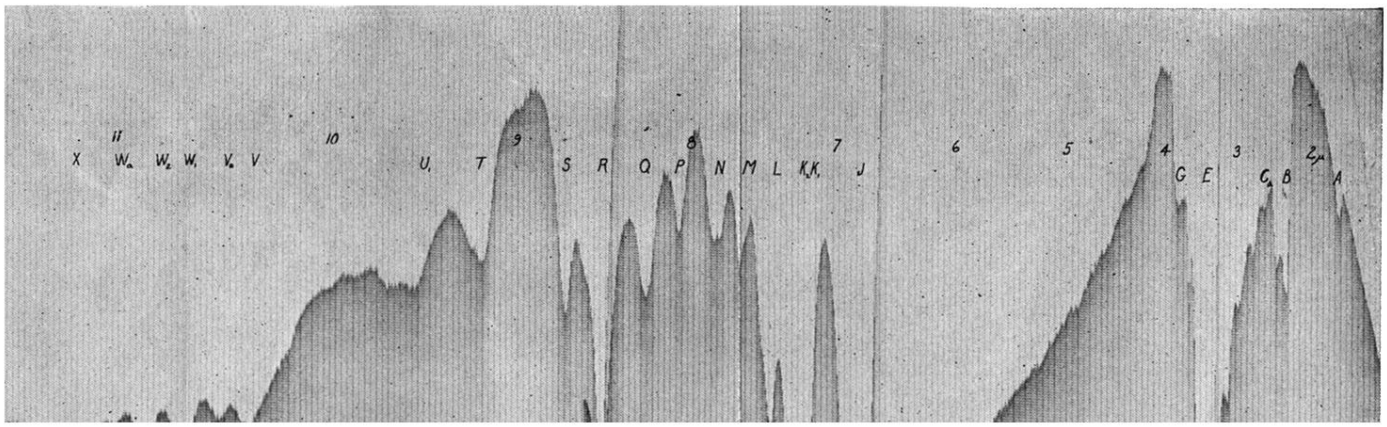
The hydrocarbons used in this work were prepared under the direction of Professor C. E. Board of the Department of Chemistry of the Ohio State University as part of the American Petroleum Institute Hydrocarbon Research Project in the Industrial Research Foundation of the University.

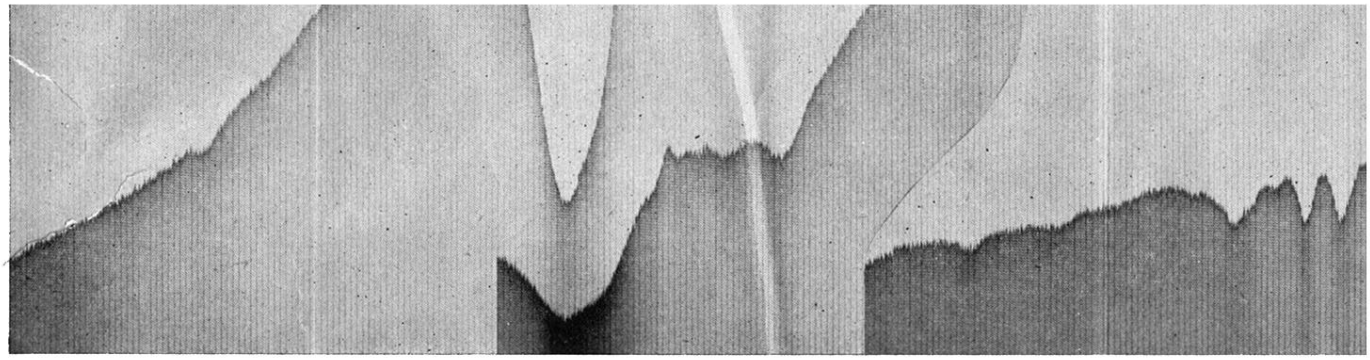
The authors also wish to express appreciation for helpful advice received from Dr. G. Calingaert and Mr. R. A. Halloran.


N-OCTANE
SOURCE: A.P.I. - No. 6-P-2
LIQUID THICKNESS 0.015 CM
AIR PATH EVACUATED
AUGUST 1, 1941 - G202 ①
15μ
14
X
W
W
13μ
W
12μ
V
II
U
T
T
T


2-METHYLHEPTANE
SOURCE: A.P.I. - No. 5-P
LIQUID THICKNESS 0.015 CM.
AIR PATH EVACUATED
AUGUST 2, 1941 - G203 ①
15μ
14
AA
Z
Z
13μ
Y
12μ
Y
II
X
W
W
W


11
10
9
8
7
6
5
4
3
2
1
U T1 T2 T
S
R1 R2 R3 R4
Q
P N M L
K1 K2 J
H
G1 G2 G3 F E
B A
O


11
10
9
8
7
6
5
4
3
2
1
X W1 W2 W3 V1 V
U1 T
S R Q P N
M L K1 K2 J
G E
C1 B
A



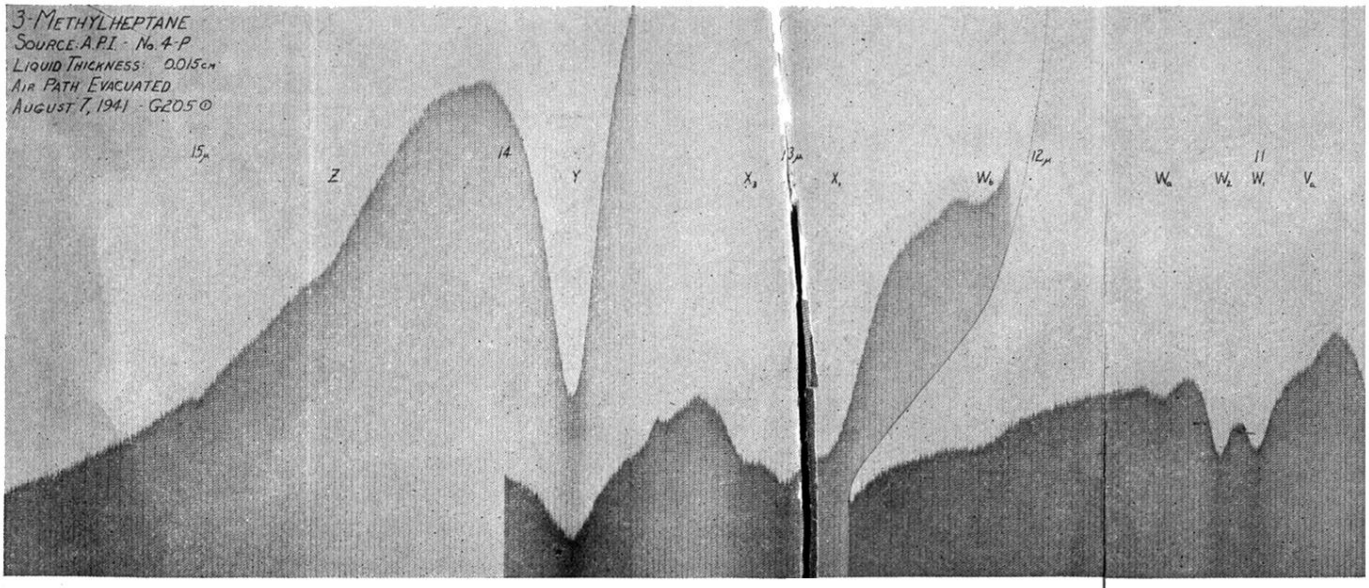
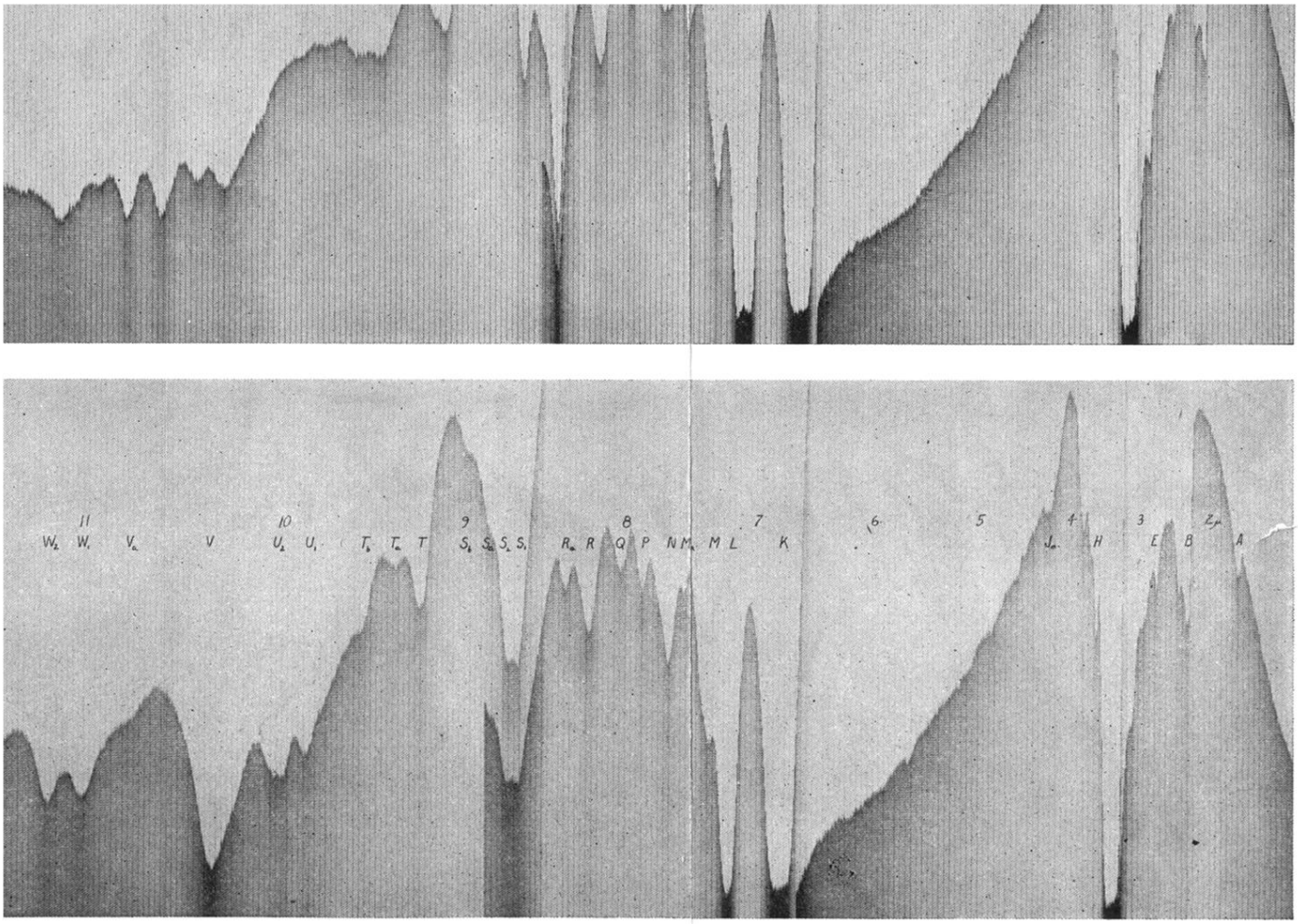


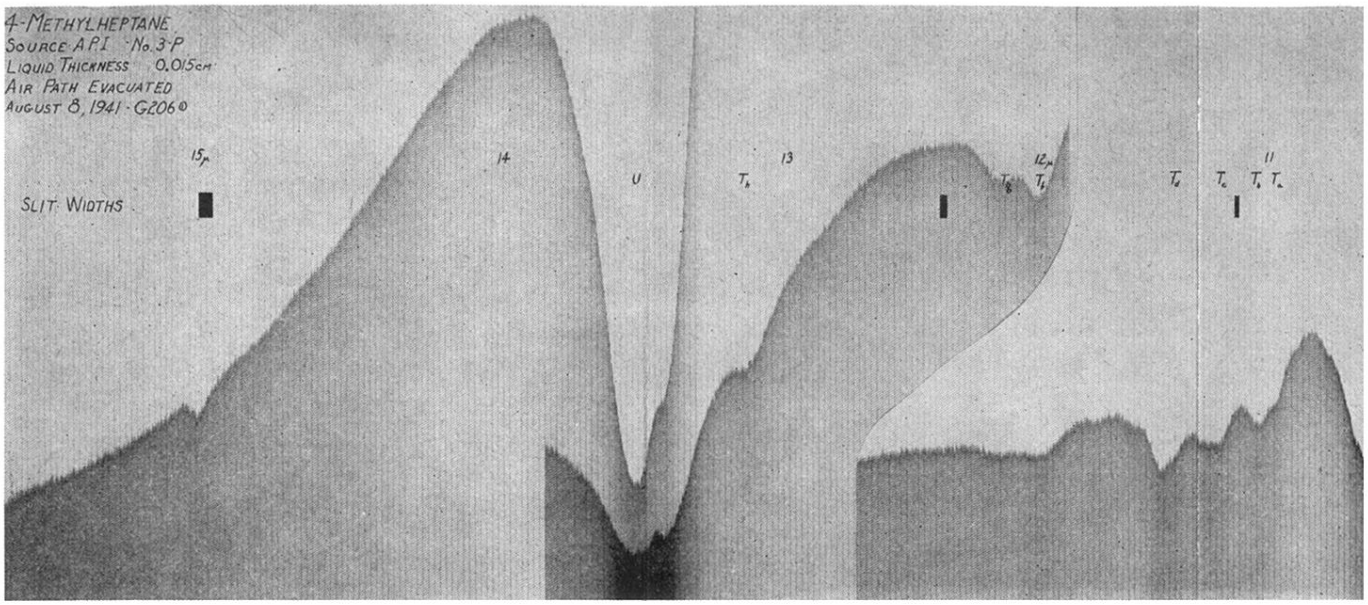
FIG. 1 (top). Infra-red spectrum of *n*-octane.

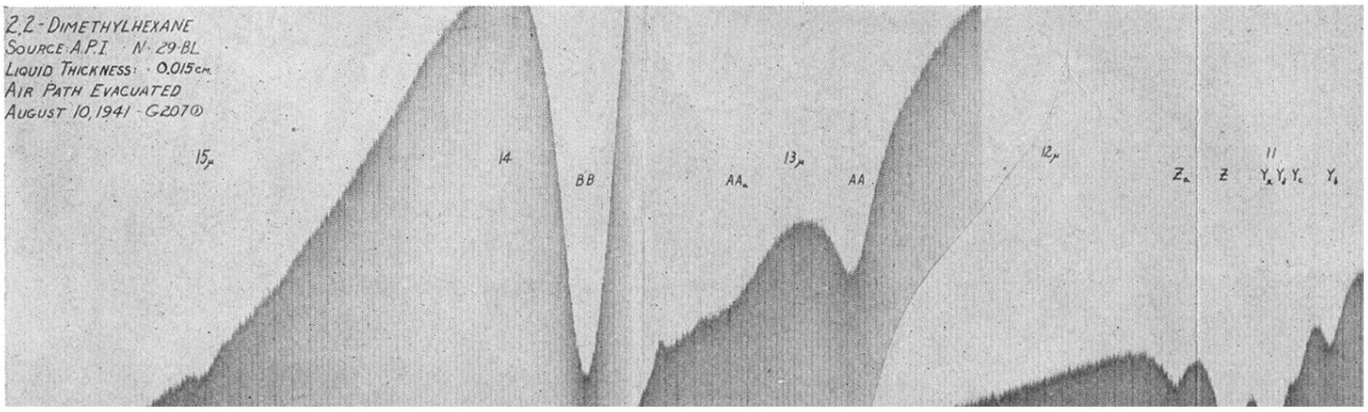
FIG. 2 (middle). Infra-red spectrum of 2-me

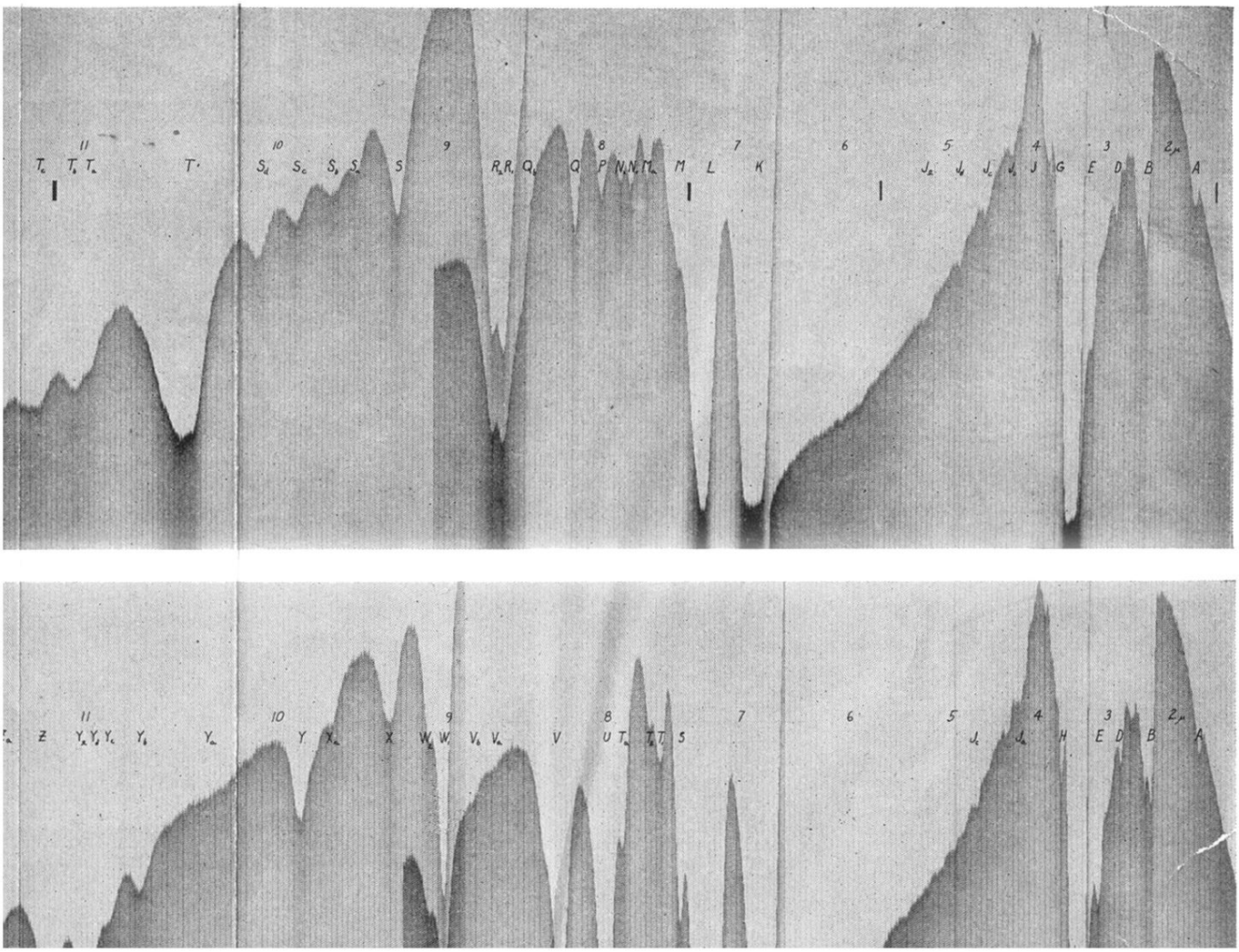


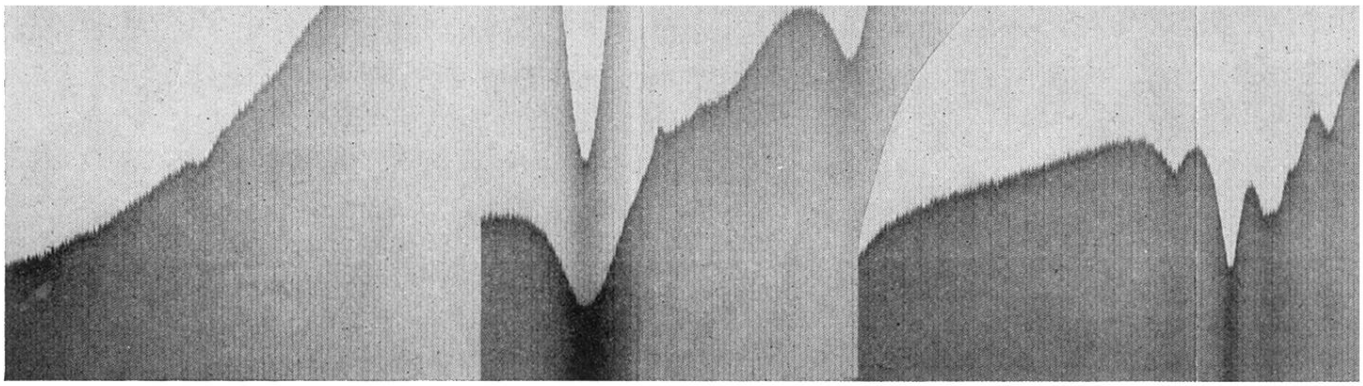
ed spectrum of 2-methylheptane.

FIG. 3 (bottom). Infra-red spectrum of 3-methylheptane.


4-METHYLHEPTANE
SOURCE A.P.I. No. 3-P
LIQUID THICKNESS 0.015cm
AIR PATH EVACUATED
AUGUST 8, 1941 - G206
SLIT WIDTHS
15μ
14
U
13
12μ
11


2,2-DIMETHYLHEXANE
SOURCE A.P.I. N-29-BL
LIQUID THICKNESS 0.015cm
AIR PATH EVACUATED
AUGUST 10, 1941 - G207
15μ
14
BB
13μ
AA
12μ
11


11
10
9
8
7
6
5
4
3
2μ
T
S
R
Q
P
N
M
L
K
J
G
E
D
B
A



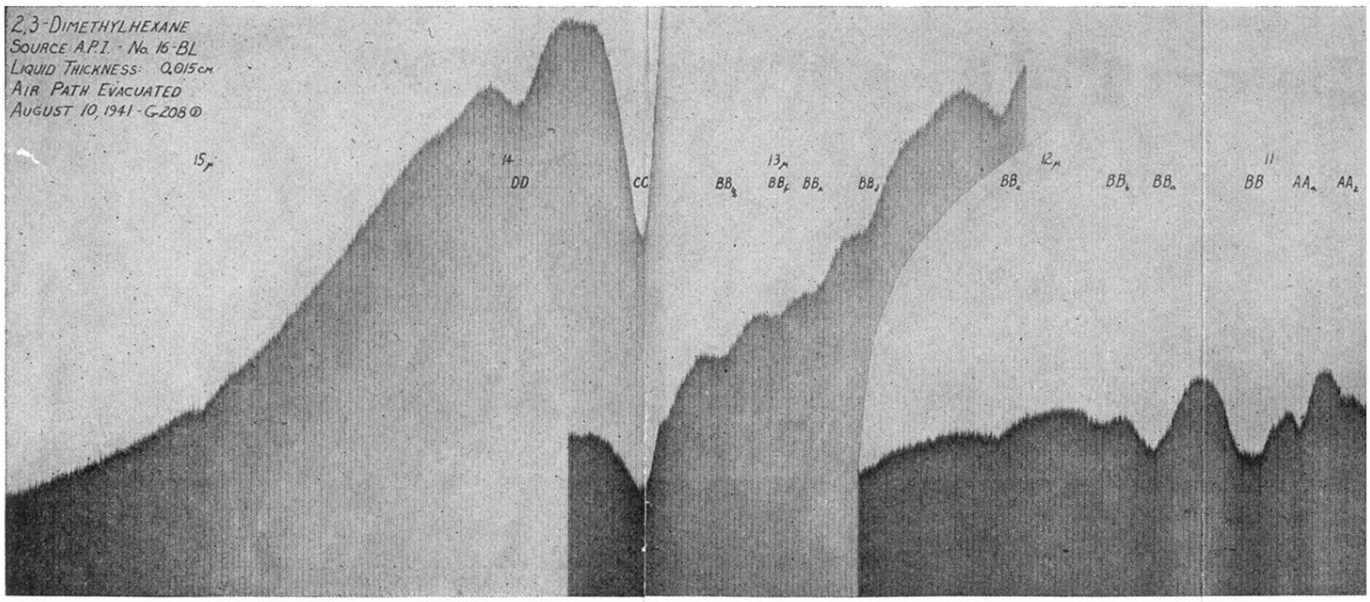
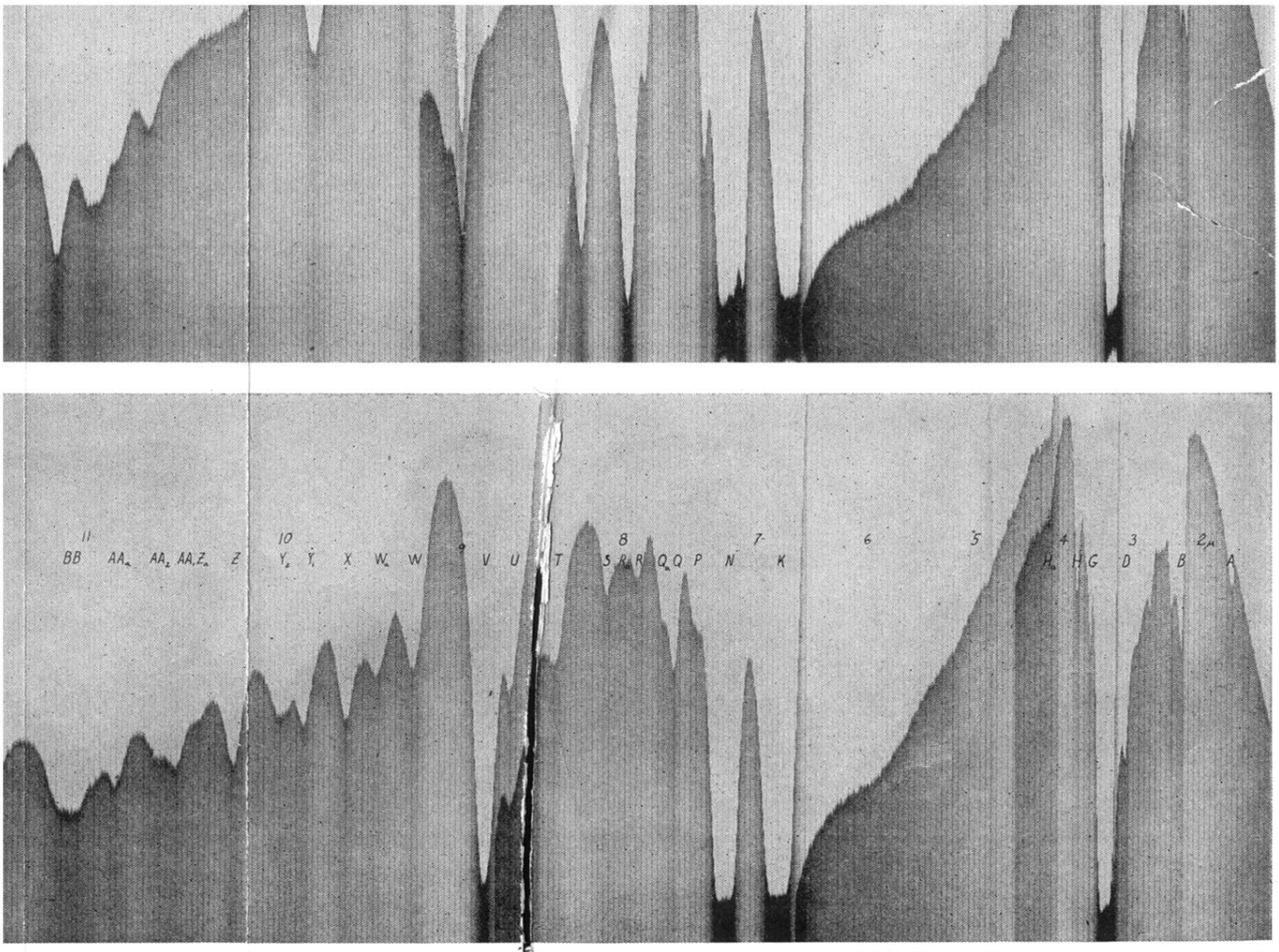


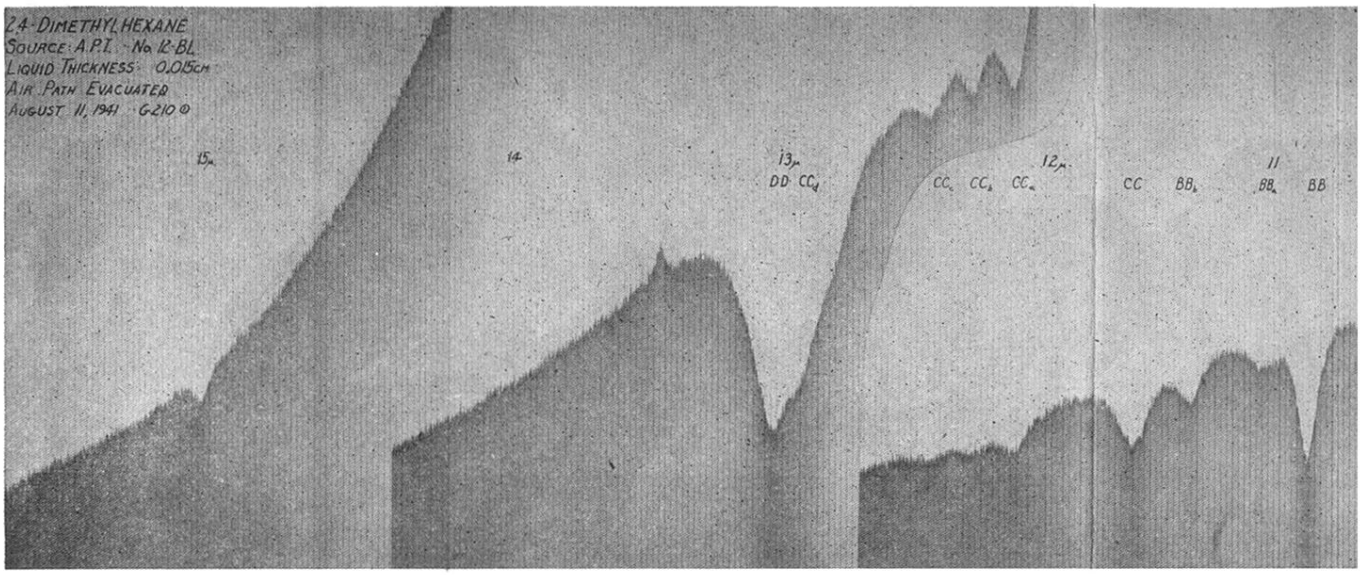
FIG. 4 (top). Infra-red spectrum of 4-methylheptane.

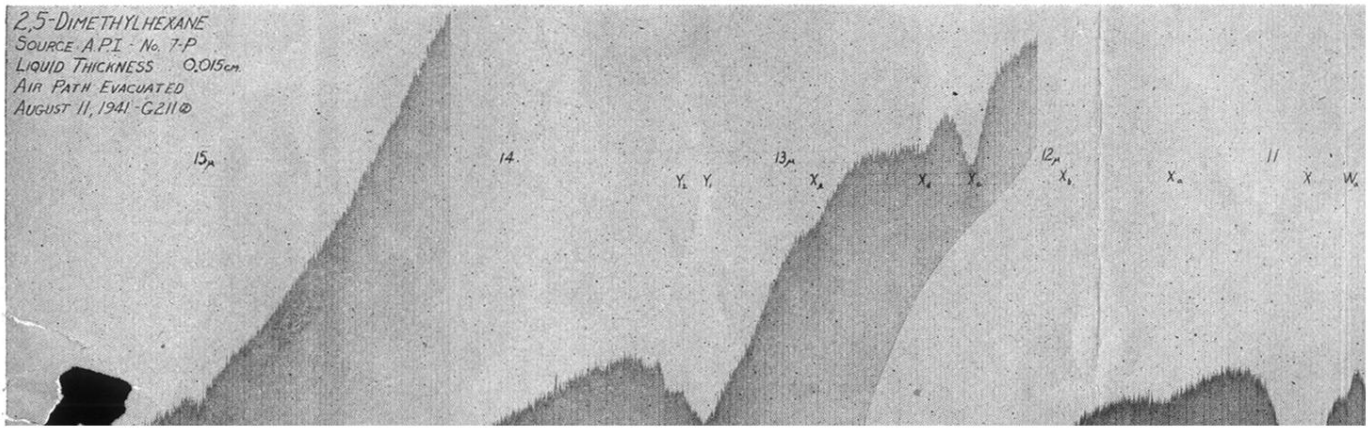
FIG. 5 (middle). Infra-red spectrum of 2,2-

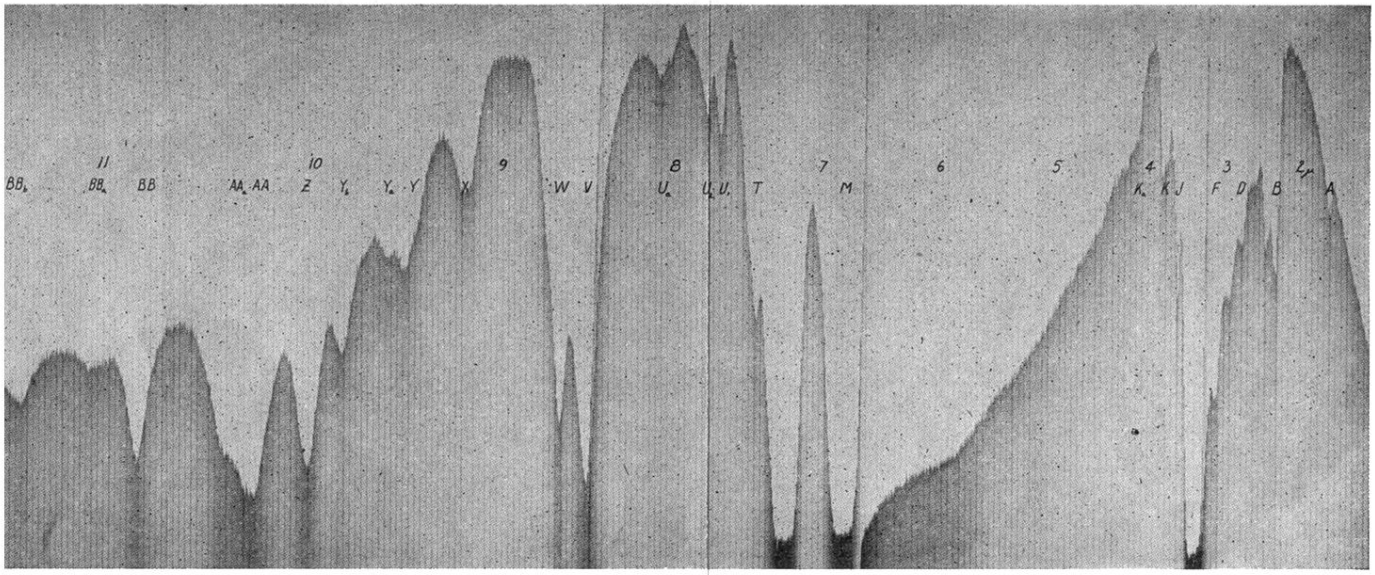


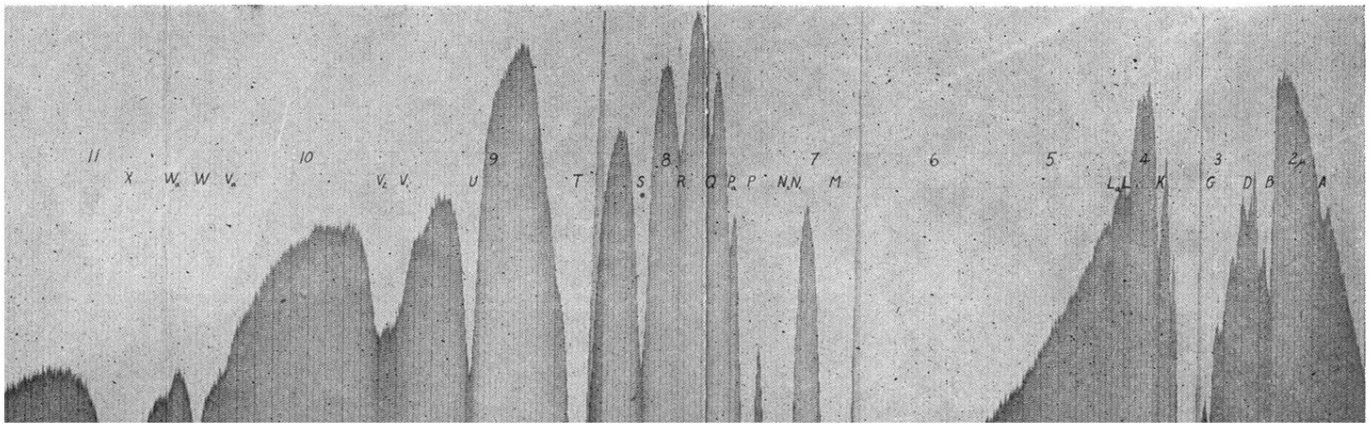
ed spectrum of 2,2-dimethylhexane.

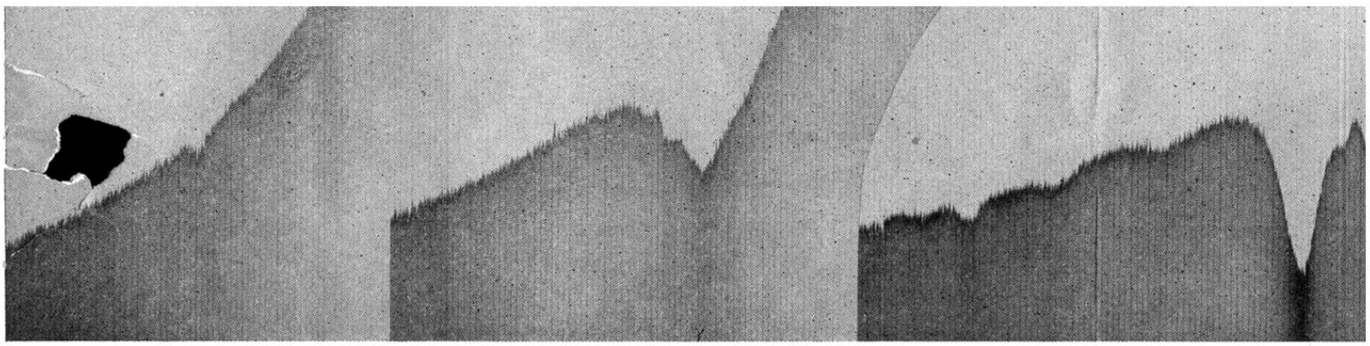
IG. 6 (bottom). Infra-red spectrum of 2,3-dimethylhexane.


2,4-DIMETHYLHEXANE
SOURCE: A.P.I. No. 12-B.L.
LIQUID THICKNESS 0.015cm
AIR PATH EVACUATED
AUGUST 11, 1941 G210
15μ
14
13μ
DD CC$_d$
12μ
CC$_c$ CC$_b$ CC$_a$
11
CC BB$_b$ BB$_a$ BB


2,5-DIMETHYLHEXANE
SOURCE: A.P.I. No. 7-P
LIQUID THICKNESS 0.015cm.
AIR PATH EVACUATED
AUGUST 11, 1941 G211
15μ
14
13μ
Y$_2$ Y$_1$ X$_4$ X$_3$ X$_2$
12μ
X$_1$
11
X$_a$ X W$_a$


11 10 9 8 7 6 5 4 3 2
BB₂ BB₁ BB AA₂ AA Z Y₂ Y₁ Y X W V U₂ U₁ U T M K K J F D B A


11 10 9 8 7 6 5 4 3 2
X W₂ W V₂ V₁ U T S R Q P₂ P N₂ N M L₂ L₁ K G D B A



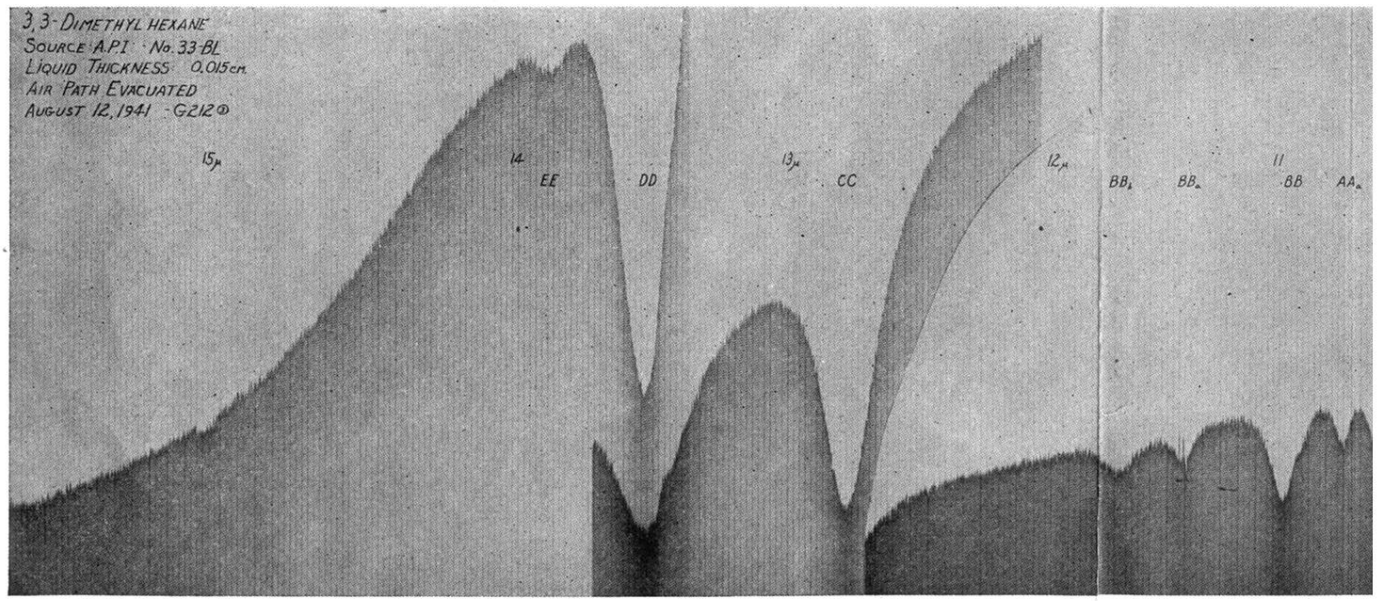
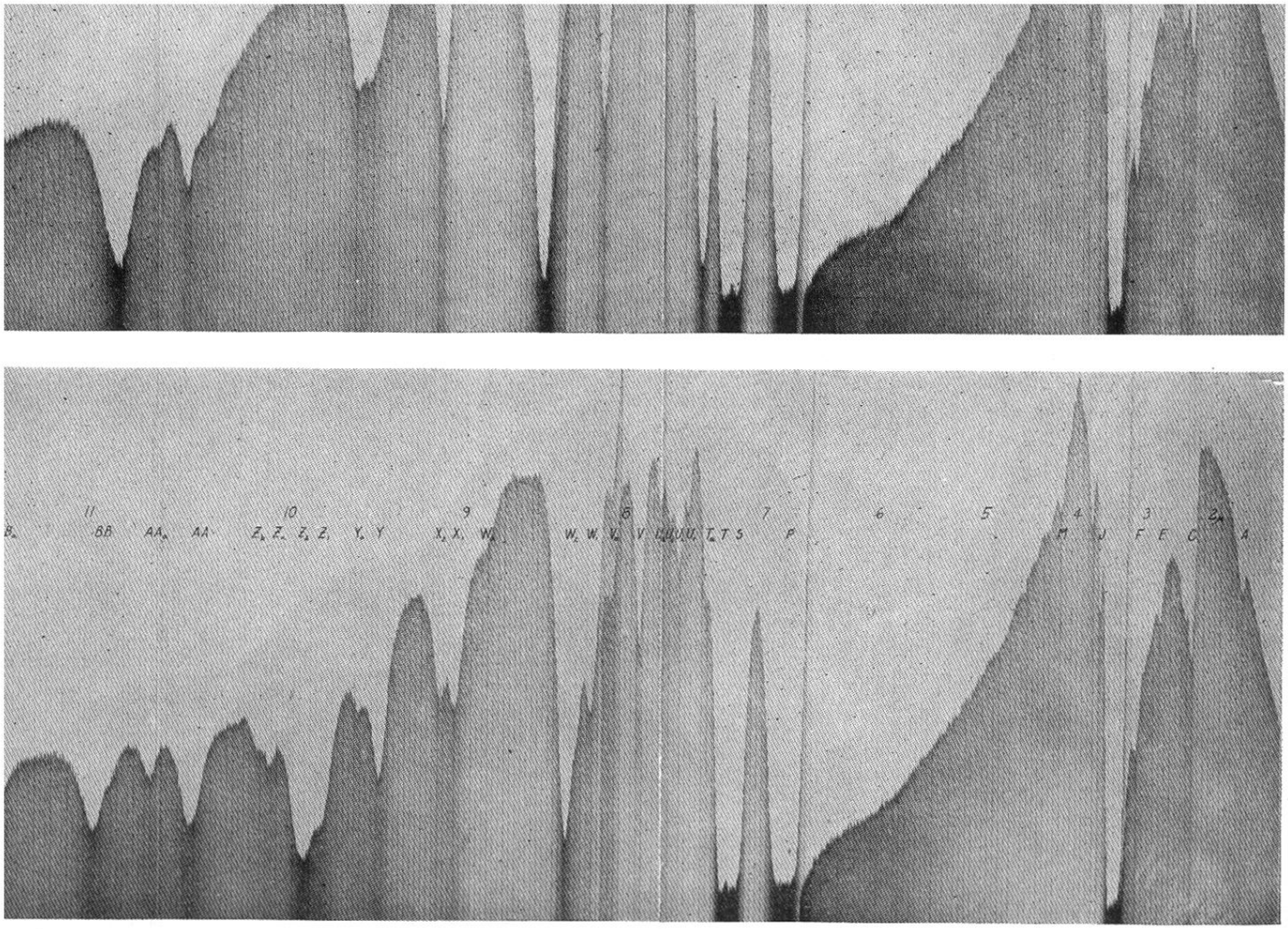


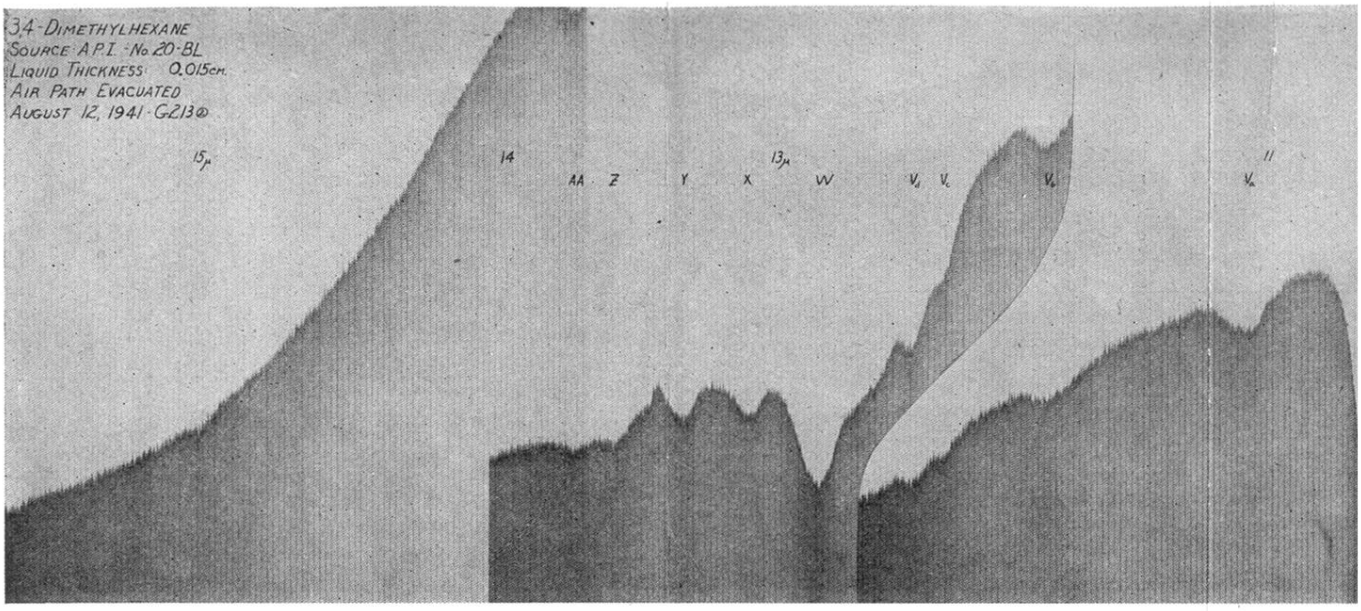
FIG. 7 (top). Infra-red spectrum of 2,4-dimethylhexane.

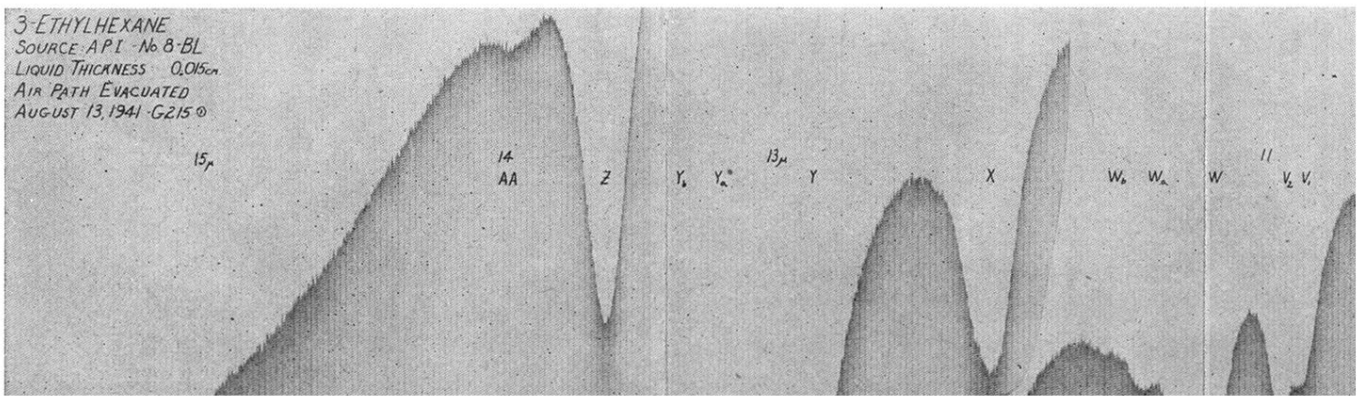
FIG. 8 (middle). Infra-red spectrum of 2,

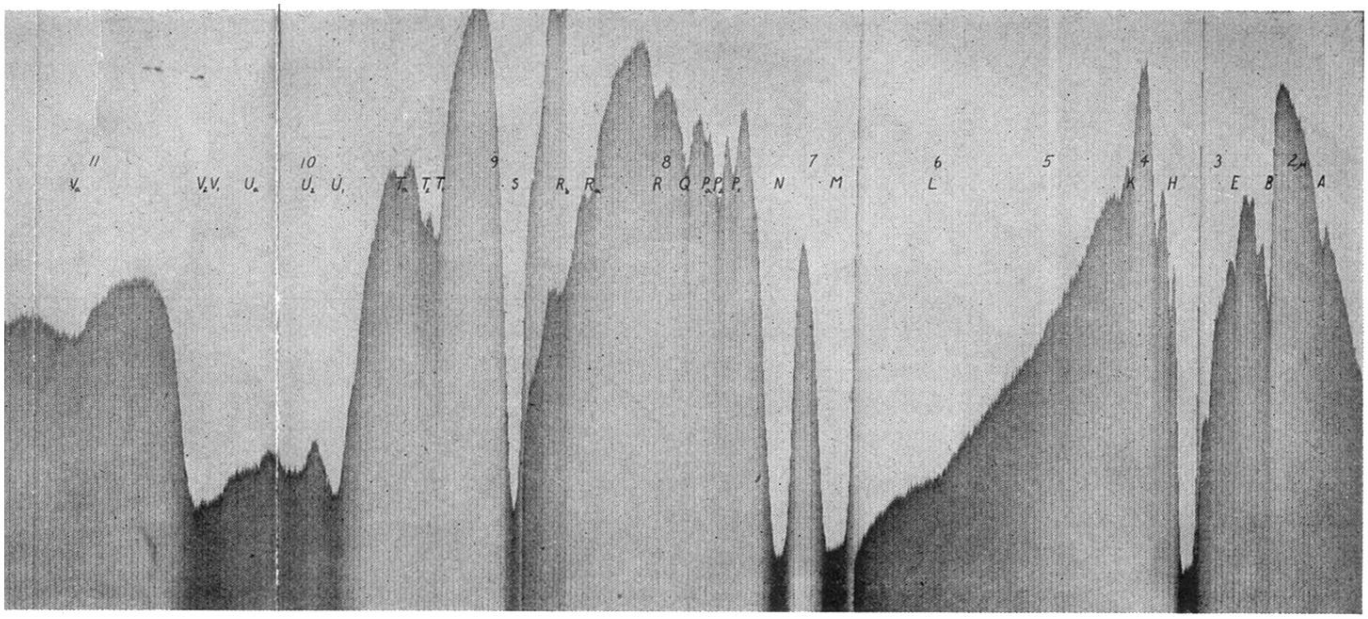


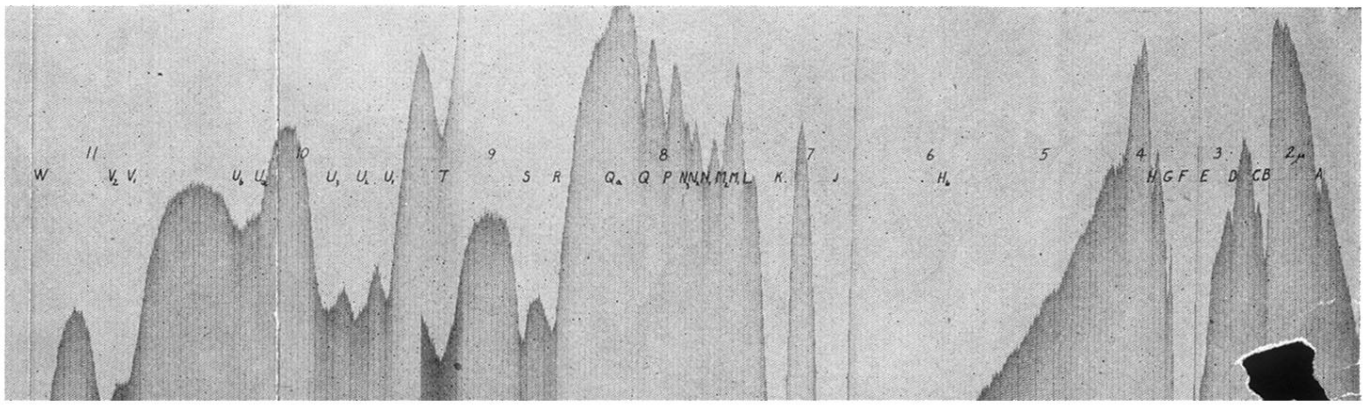
·red spectrum of 2,5-dimethylhexane.

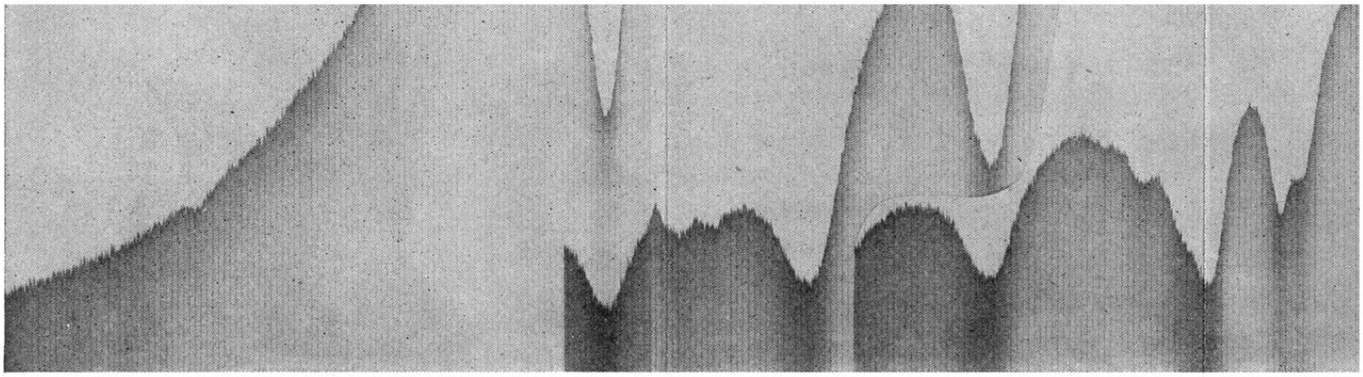
FIG. 9 (bottom). Infra-red spectrum of 3,3-dimethylhexane.


3,4-DIMETHYLHEXANE
SOURCE: A.P.I. - No. 20-BL
LIQUID THICKNESS 0.015cm.
AIR PATH EVACUATED
AUGUST 12, 1941 - G213®
15μ
14
AA
Z
Y
X
13μ
W
V1
Vc
Vb
11
Va


3-ETHYLHEXANE
SOURCE: A.P.I. - No. 8-BL
LIQUID THICKNESS 0.015cm.
AIR PATH EVACUATED
AUGUST 13, 1941 - G215®
15μ
14
AA
Z
Yb
Ya
13μ
Y
X
Wb
Wa
W
11
V2
V1


11 10 9 8 7 6 5 4 3 2 1
V1 V2 V3 U4 U3 U2 U1 T4 T3 T2 T1 S R3 R2 R1 R Q P3 P2 P1 P N M L K H E B A


11 10 9 8 7 6 5 4 3 2 1
W V2 V1 U4 U3 U2 U1 T S R Q3 Q P N4 N3 N2 N1 M3 M2 M1 L K J H3 H2 H1 G F E D C B A



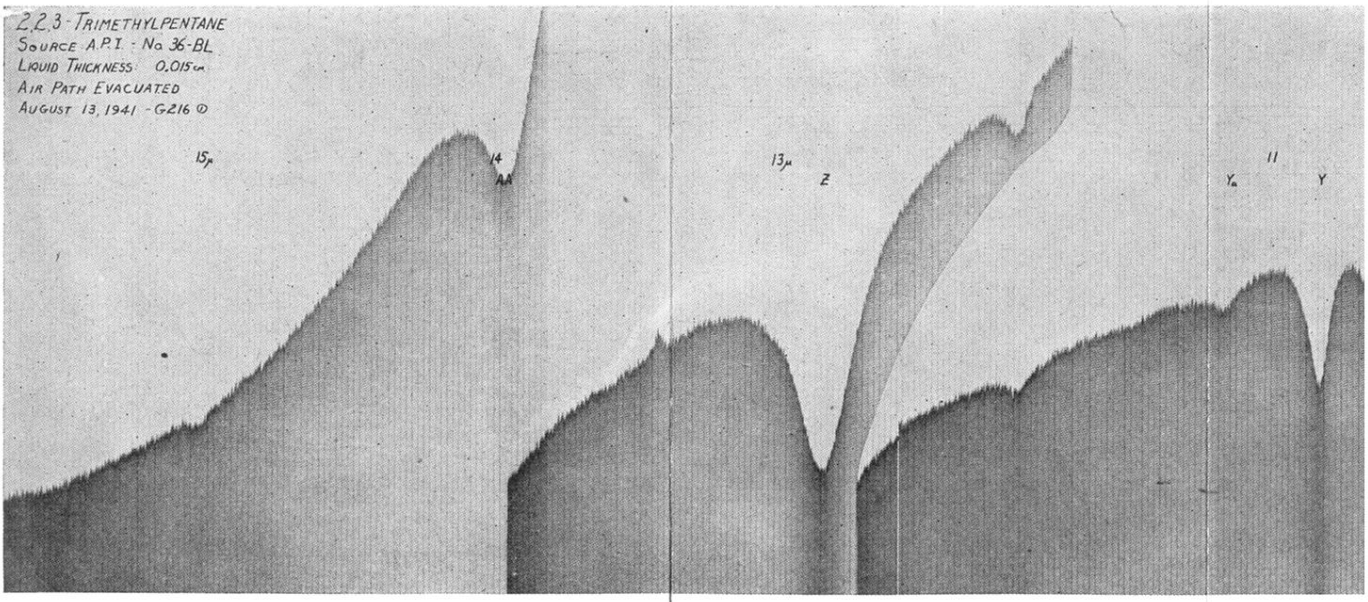
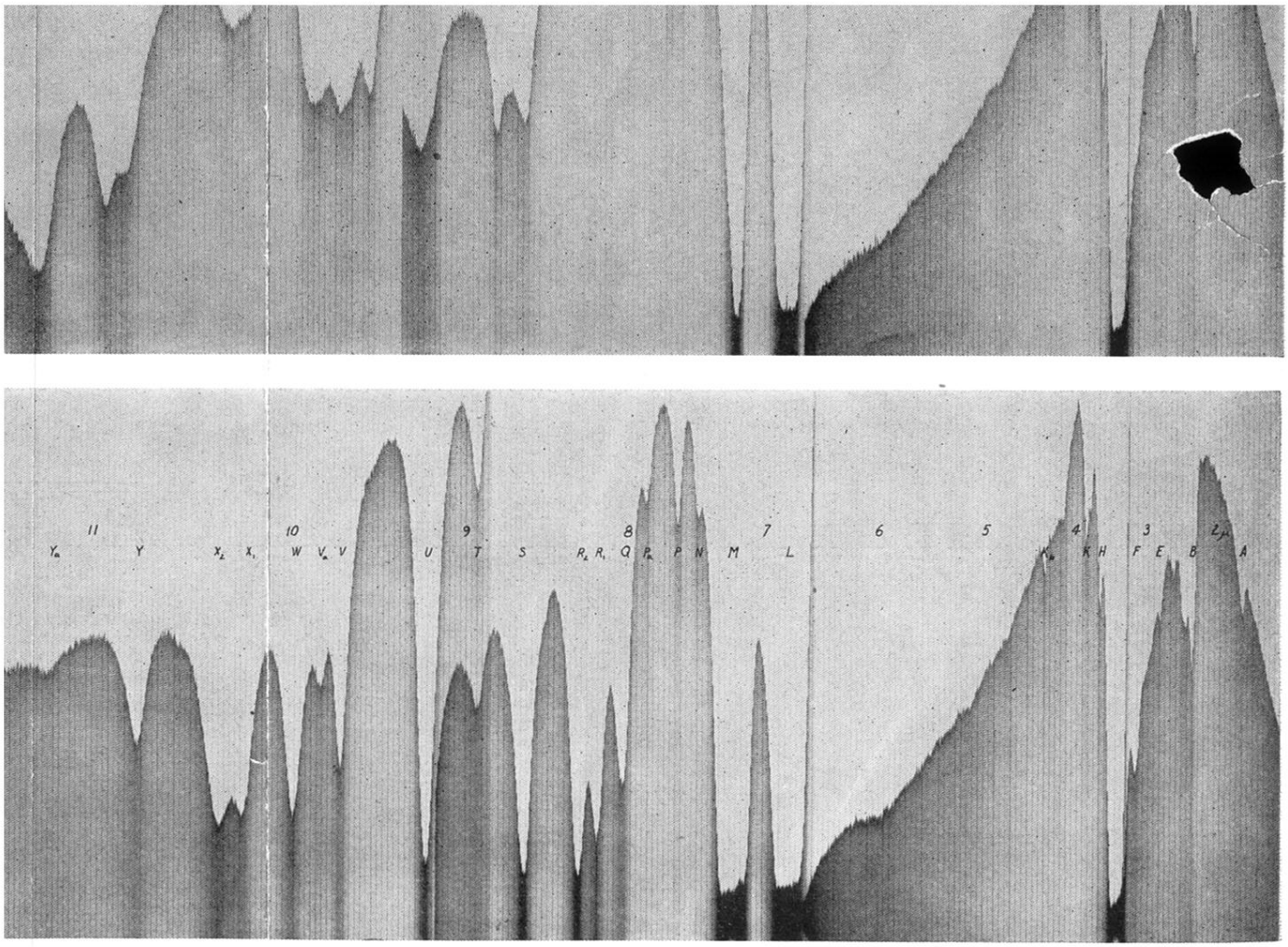


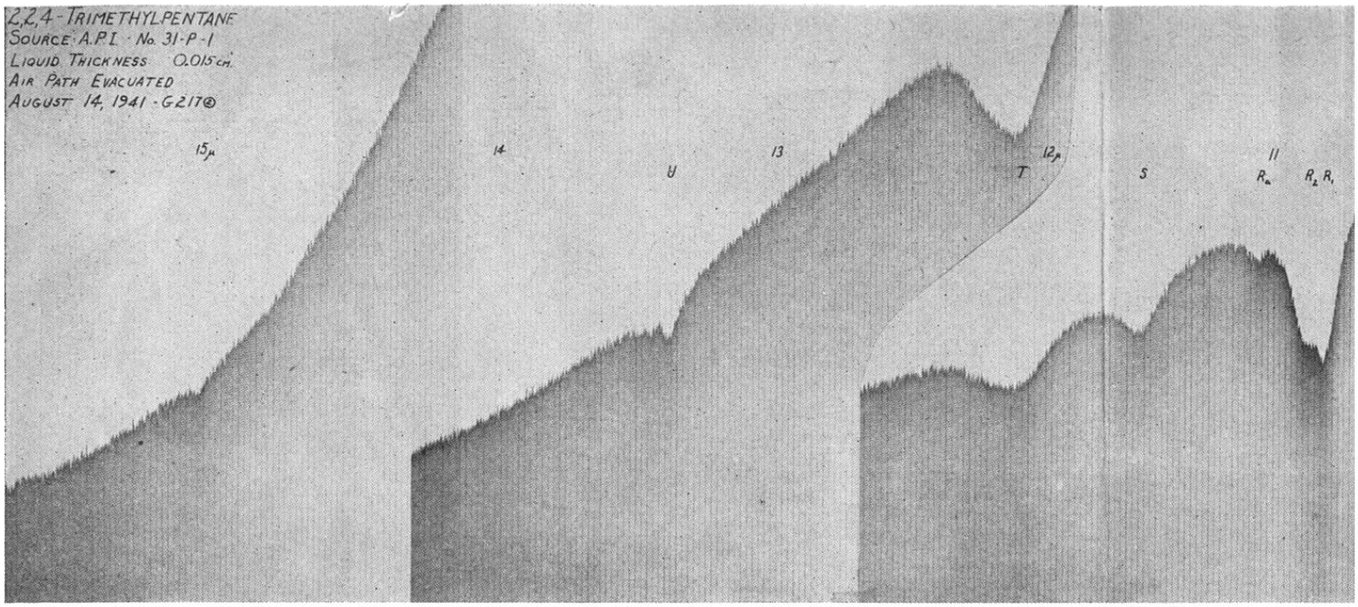
FIG. 10 (top). Infra-red spectrum of 3,4-dimethylhexane.

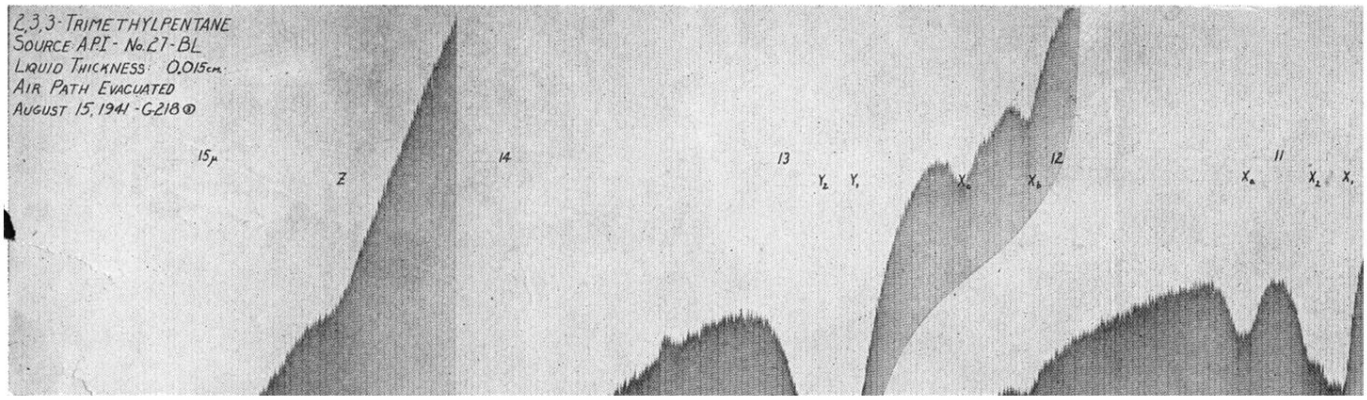
FIG. 11 (middle). Infra-red spectrum of

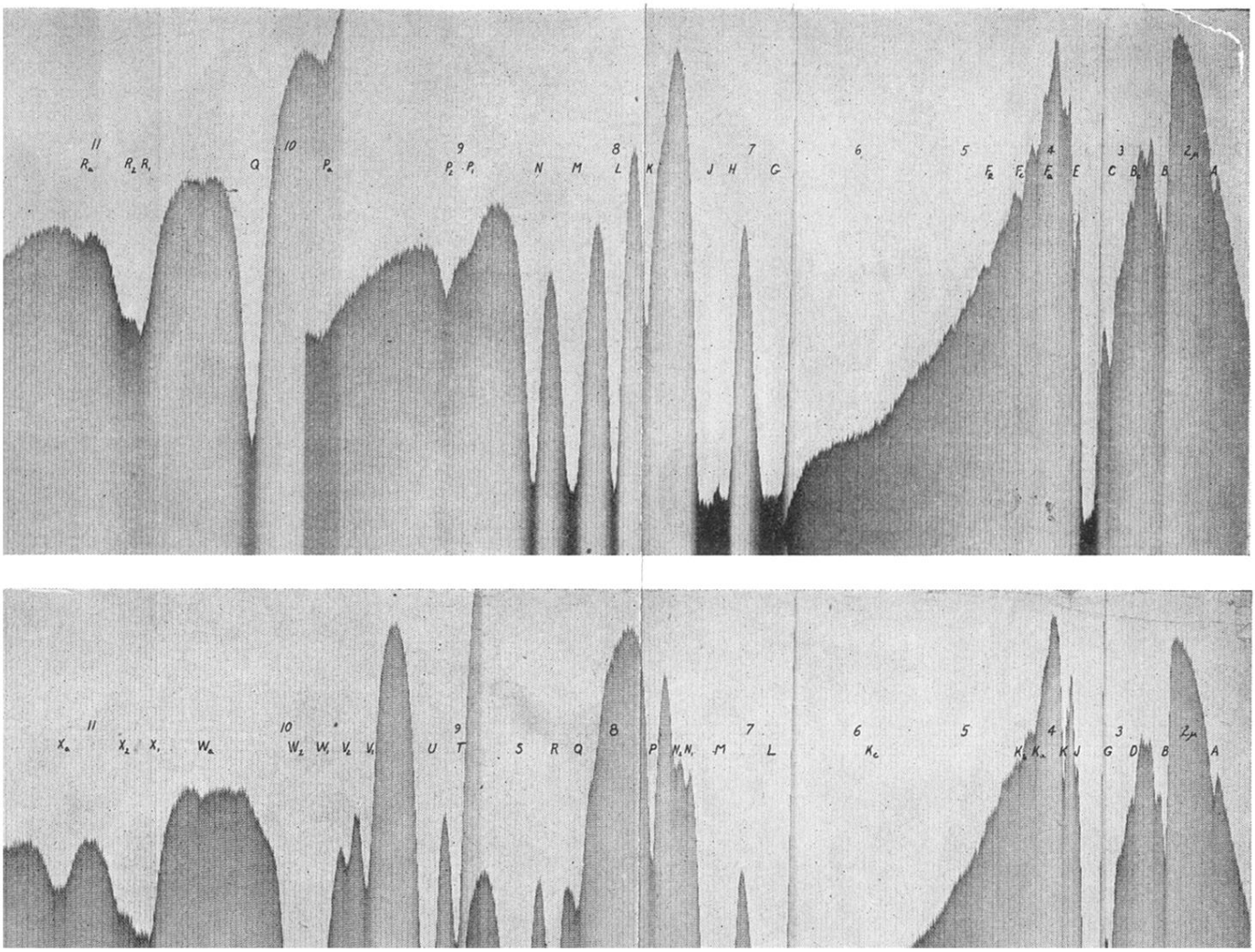


·a-red spectrum of 3-ethylhexane.

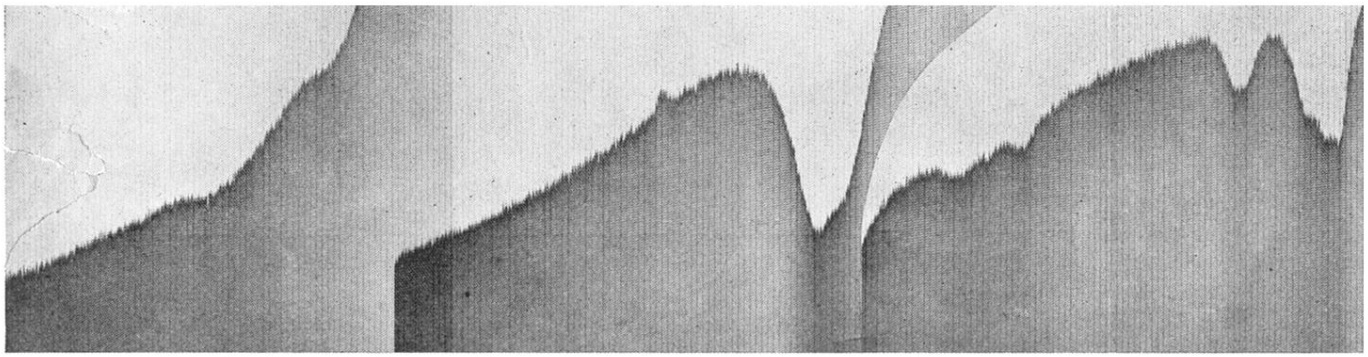
FIG. 12 (bottom). Infra-red spectrum of 2,2,3-trimethylpentane.


2,2,4-TRIMETHYLPENTANE
SOURCE: A.P.I. : No. 31-P-1
LIQUID THICKNESS: 0.015 cm.
AIR PATH EVACUATED
AUGUST 14, 1941 - G-217 ①
15μ
14
U
13
12μ
T
S
11
R₂
R₁


2,3,3-TRIMETHYLPENTANE
SOURCE: A.P.I. - No. 27-B.L.
LIQUID THICKNESS: 0.015 cm.
AIR PATH EVACUATED
AUGUST 15, 1941 - G-218 ①
15μ
Z
14
13
Y₂
Y₁
12
11
X₂
X₁


11
R_a R_2 R_1
Q
10
P_a
9
P_2 P_1
N M
8
L
K
7
J H
G
6
5
F_2 F_1
4
F_a E
3
C B_a
B
2
A

11
X_a X_2 X_1 W_a
10
W_2 W_1 V_2 V_1
9
U T
S R Q
8
P
7
N_2 N_1 M
L
6
K_c
5
K_b K_a
4
K J
3
G D
B
2
A



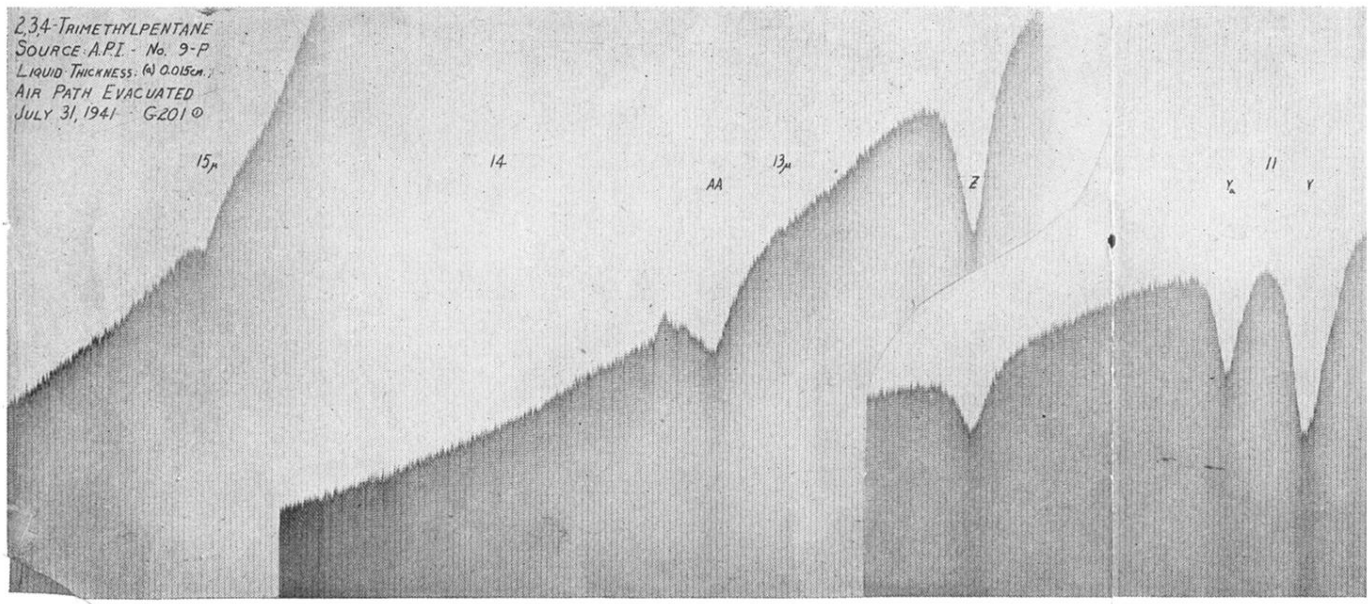
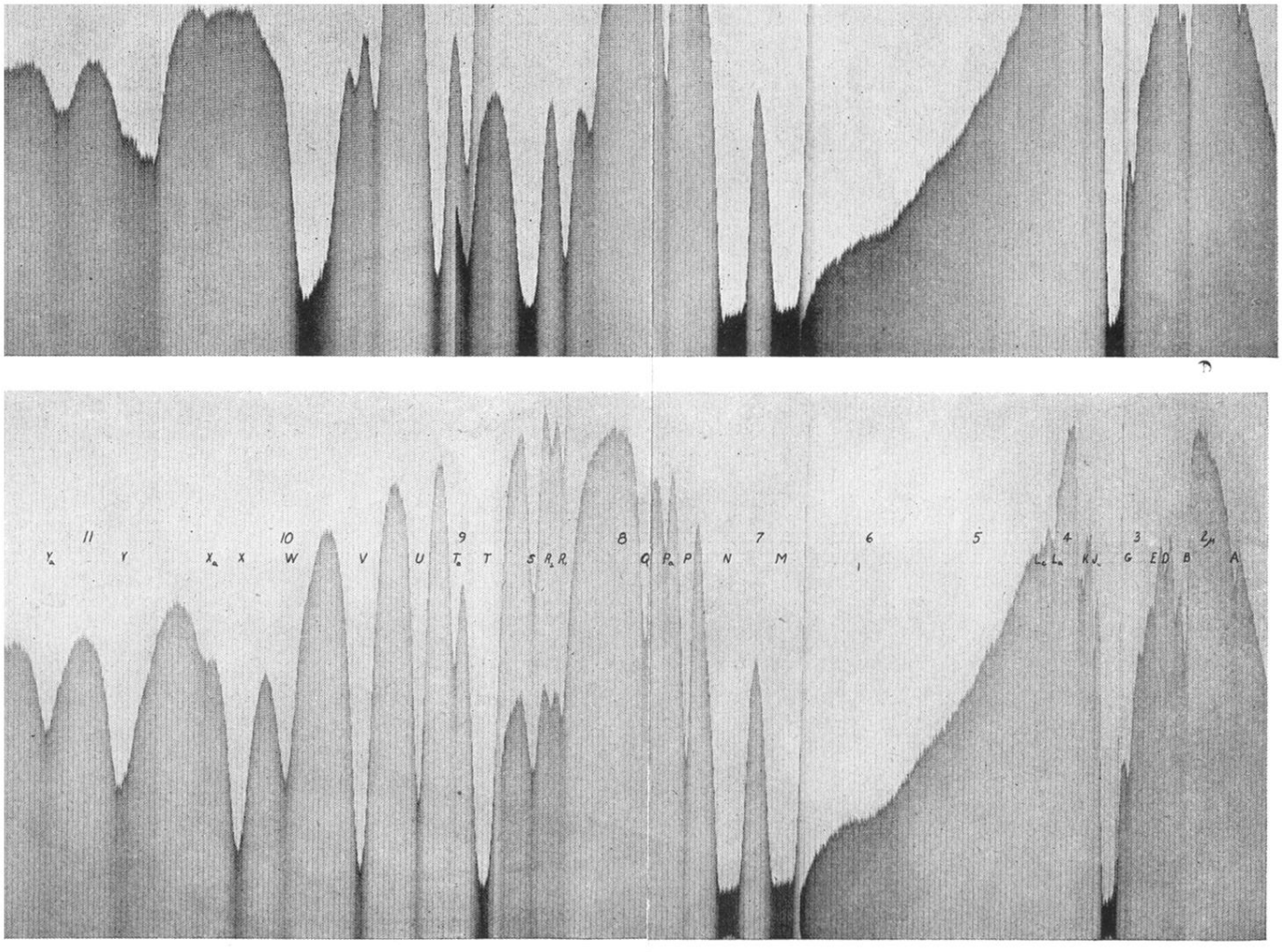


FIG. 13 (top). Infra-red spectrum of 2,2,4-trimethylpentane.

FIG. 14. (middle) Infra-red spectrum of 2,3,



ed spectrum of 2,3,3-trimethylpentane.

FIG. 15 (bottom). Infra-red spectrum of 2,3,4-trimethylpentane.

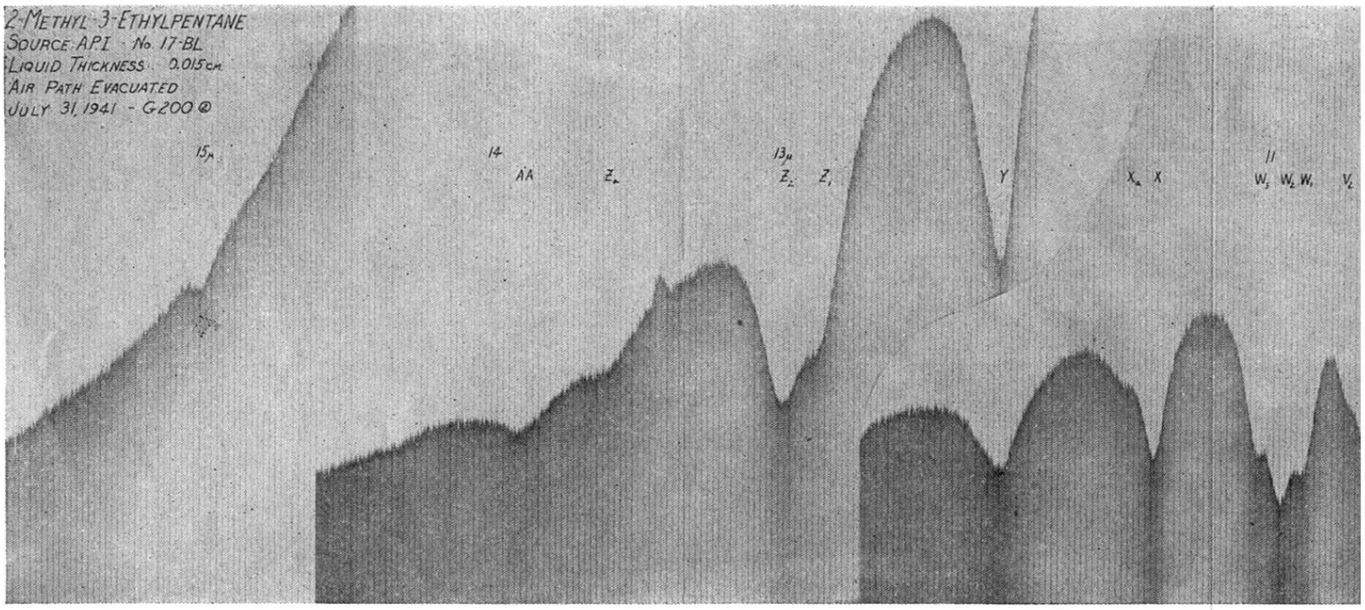


FIG. 16. Infra-red spectrum of 2-meth

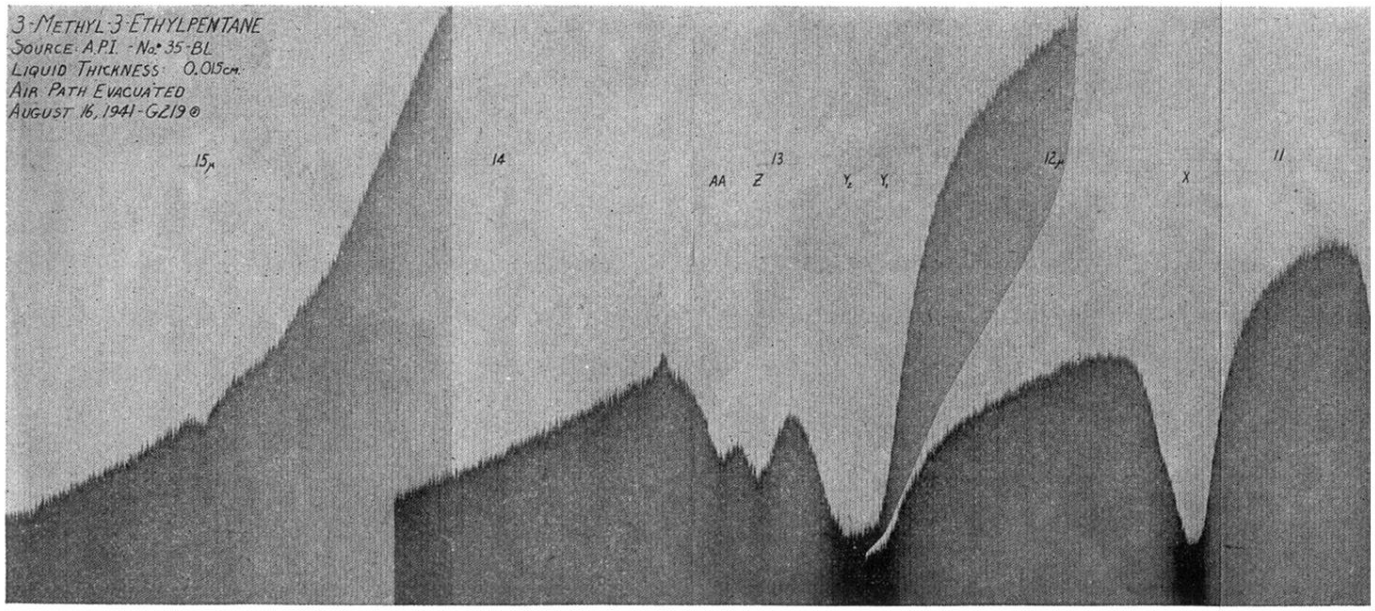
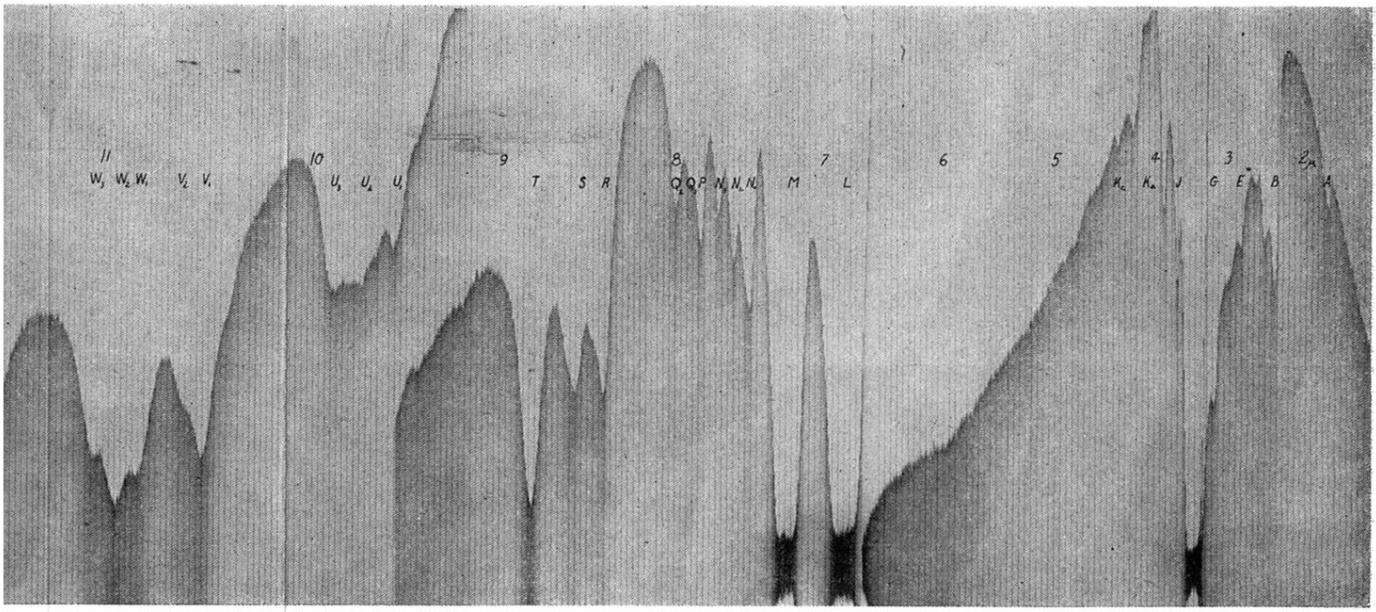
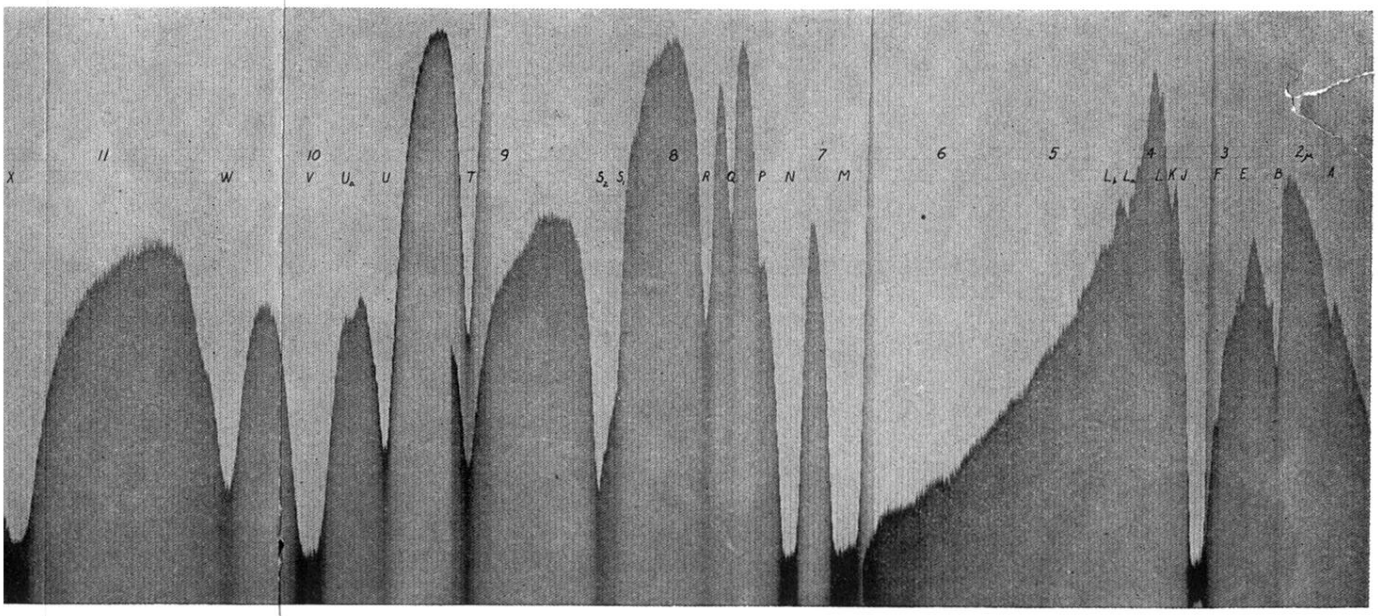


FIG. 17. Infra-red spectrum of 3-meth



spectrum of 2-methyl, 3-ethylpentane.



spectrum of 3-methyl, 3-ethylpentane.