

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

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THIS is a continuation of the preceding paper¹ having been given in that paper, and data for the octanes in the liquid for the octanes in the vapor phase here.

TABLE I.

<i>n</i> -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})
A	2.317	4316	A	1.704	5869	A	1.697	5893	A	1.682	5945	A	1.682	5945
B	2.451	4080	B	2.338	4277	B	2.300	4348	B	2.313	4323	B	2.323	4305
C	3.154	3171	C	2.443	4093	C	2.439	4100	C	2.443	4093	C	2.403	4161
D	3.441	2906	D	3.146	3179	D	2.580	3876	D*	2.774	3605	D*	2.790	3584
E	3.658	2734	E	3.433	2913	E*	2.774	3605	E	3.140	3185	E	3.143	3182
F	3.731	2680	F	3.660	2732	F	3.145	3180	F	3.428	2917	F	3.424	2921
G	3.869	2585	G	3.793	2637	G	3.436	2910	G	3.653	2737	G	3.674	2722
H	6.819	1466	H	4.314	2318	H	3.648	2741	H	3.826	2614	J	3.930	2545
J	7.219	1385	J	6.809	1469	J	3.820	2618	K	3.985	2509	L	6.784	1474
K	7.410	1350	K	7.221	1385	K	6.820	1466	L	6.814	1468	Q	7.286	1372
L	7.655	1306	L	7.427	1346	L	7.221	1385	M	7.212	1387	S	7.458	1341
M	7.852	1274	M	7.628	1311	M	7.384	1354	N	7.445	1343	T	7.620	1312
N	8.135	1229	N	7.805	1281	N	7.652	1307	N	7.800	1282	U	7.975	1254
P	8.315	1203	P	8.031	1245	P	7.840	1276	P	7.960	1256	V	8.296	1206
Q	8.774	1140	Q	8.238	1214	Q	7.990	1251	Q	8.148	1227	W	9.069	1103
R	9.248	1081	R	8.534	1172	R	8.201	1219	R	8.635	1158	X	9.370	1067
S	10.305	970	S	8.719	1147	S	8.666	1154	S	9.289	1076	Y	9.835	1017
T	10.926	915	T	9.210	1086	T	9.228	1084	T	10.482	954	Z	11.109	900
U	11.345	882	U	9.577	1044	U	9.986	1001	U	13.479	742	AA	12.694	788
V	11.806	847	V	10.391	962	V	10.338	967				BB	13.645	733
W	13.015	768	W	10.699	935	W	11.080	903						
X	13.832	723	X	11.153	896	X	12.846	778						
			Y	11.902	840	Y	13.710	729						
			Z	12.986	770									
			AA	13.759	727									

2,3-Dimethylhexane			2,4-Dimethylhexane			2,5-Dimethylhexane			3,3-Dimethylhexane			3,4-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})
A	1.694	5903	A	1.715	5831	A	1.690	5917	A	1.688	5924	A	1.703	5872
B	2.323	4305	B	2.339	4275	B	2.331	4290	B	1.873	5339	B	2.305	4338
C	2.449	4083	C	2.460	4065	C	2.443	4093	C	2.317	4316	C	2.446	4088
D	3.154	3171	D*	2.780	3597	D	2.628	3805	D	2.438	4102	D	2.600	3846
E	3.443	2913	E	2.968	3369	E*	2.773	3606	E*	2.779	3598	E*	2.777	3601
F	3.657	2734	F	3.149	3176	F	2.964	3374	F	3.150	3175	F	3.159	3166
G	3.837	2606	G	3.442	2905	G	3.137	3188	G	3.427	2918	G	3.429	2916
H	6.815	1467	J	3.665	2729	H	3.440	2907	J	3.653	2737	H	3.648	2741
K	7.226	1384	K	3.867	2586	J	3.658	2734	K	3.784	2643	J	3.830	2611
L	7.454	1342	M	6.804	1470	K	3.809	2625	L	3.913	2556	K	4.154	2407
M	7.626	1311	R	7.247	1380	L	4.200	2381	M	4.299	2326	L	6.043	1655
N	7.863	1272	T	7.450	1342	M	6.789	1473	P	6.806	1469	M	6.828	1465
O	8.043	1243	U	7.750	1290	N	7.230	1383	S	7.246	1380	N	7.229	1383
P	8.454	1183	V	8.544	1170	P	7.441	1344	U	7.614	1313	P	7.617	1313
Q	8.664	1154	W	8.638	1158	Q	7.696	1299	V	7.896	1266	Q	7.847	1274
R	8.845	1131	X	9.227	1084	R	7.902	1266	W	8.339	1199	R	8.030	1245
S	9.299	1076	Y	9.536	1049	S	8.139	1229	X	9.093	1100	S	8.885	1125
T	9.636	1038	Z	10.026	998	T	8.527	1173	Y	9.506	1052	T	9.348	1070
U	9.930	1008	AA	10.300	971	U	9.164	1091	Z	9.867	1014	U	9.867	1014
V	10.248	976	BB	10.836	923	V	9.563	1046	AA	10.480	954	V	10.434	958
W	10.582	945	CC	11.605	862	W	10.475	955	BB*	10.944	914	W	12.793	782
X	11.064	904	DD	12.967	771	X	10.844	922	CC	12.779	783			
Y	13.591	736				Y	13.326	750	DD	13.492	741			

* Probably due to impurity in sodium chloride prism.

* 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 Review of Scientific Instruments **13**, 515 (1942). The second paper is published immediately preceding this one.

** Now at the Beacon Research Laboratory of the Texas Company, Beacon, New York.

¹ R. A. Oetjen, H. M. Randall, and W. E. Anderson, Rev. Mod. Phys. **16**, 260 (1944).

TABLE I.—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	1.676	5967	A	1.684	5938	A	1.688	5924	A	1.694	5903
B	2.300	4348	B	2.303	4342	B	2.310	4329	B	2.300	4348	B	2.308	4333
C	2.435	4107	C	2.393	4179	C	3.135	3190	C	2.423	4127	C	2.453	4073
D*	2.773	3606	D	2.577	3880	D	3.433	2913	D	2.578	3879	D	2.628	3805
E	3.152	3173	E*	2.783	3593	E	3.669	2726	E*	2.778	3600	E*	2.780	3597
F	3.435	2911	F	3.139	3186	F	3.793	2636	F	2.984	3351	F	2.961	3377
G	3.643	2745	G	3.429	2916	G	6.783	1474	G	3.145	3180	G	3.154	3171
H	3.855	2594	H	3.655	2736	H	7.168	1395	H	3.410	2933	H	3.433	2913
J	6.828	1465	J	3.786	2641	J	7.298	1370	J	3.645	2743	J	3.657	2734
K	7.209	1387	K	3.846	2600	K	7.758	1289	K	3.825	2614	K	3.808	2626
L	7.442	1344	L	6.787	1473	L	7.987	1252	L	6.806	1469	L	3.862	2589
M	7.616	1313	M	7.248	1380	M	8.273	1209	M	7.228	1384	M	6.805	1470
N	7.779	1286	N	7.465	1340	N	8.524	1173	N	7.494	1334	N	7.225	1384
P	7.979	1253	P	7.635	1310	P	9.055	1104	P	7.698	1299	P	7.555	1324
Q	8.116	1232	Q	8.019	1247	Q	10.181	982	Q	8.215	1217	Q	7.839	1276
R	8.676	1153	R	8.267	1210	R	10.775	928	R	8.383	1193	R	8.430	1186
S	8.824	1133	S	8.641	1157	S	11.610	861	S	8.626	1159	S	8.573	1166
T	9.278	1078	T	8.968	1115	T	12.052	830	T	9.016	1109	T	8.900	1124
U	9.742	1026	U	9.234	1083				U	9.164	1092	U	9.276	1078
V	10.878	919	V	9.732	1027				V	9.586	1044	V	9.600	1042
W	11.273	887	W	9.966	1004				W	9.875	1012	W	10.012	999
X	12.133	824	X	10.276	973				X	10.771	928	X	10.251	976
Y	12.872	777	Y	10.788	927				Y	12.845	779	Y	10.848	922
Z	13.610	735	Z	12.835	779							Z	12.284	814
AA			AA	13.986	715									

2-Methyl, 3-ethylpentane			2-Methyl, 3-ethylpentane			3-Methyl, 3-ethylpentane			3-Methyl, 3-ethylpentane			2,2,3,3-Tetramethylbutane		
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	1.691	5914	P	7.838	1276	A	1.702	5875	P	7.440	1344	A	1.676	5967
B	2.304	4340	Q	7.960	1256	B	2.302	4344	Q	7.620	1312	B	2.313	4323
C	2.440	4098	R	8.445	1184	C	2.439	4100	R	7.784	1285	C	2.408	4153
D	2.592	3858	S	8.584	1165	D	2.538	3940	S	8.427	1187	D	2.583	3871
E*	2.777	3601	T	8.848	1130	E*	2.788	3587	T	9.207	1086	E*	2.770	3610
F	2.922	3422	U	9.718	1029	F	3.149	3176	U	9.637	1038	F	2.894	3455
G	3.156	3169	V	10.560	947	G	3.243	3084	V	10.008	999	G	2.970	3367
H	3.429	2916	W	10.912	916	H	3.419	2925	W	10.408	960	H	3.100	3226
J	3.644	2744	X	11.509	869	J	3.631	2754	X	11.366	880	J	3.404	2938
K	3.823	2616	Y	12.118	825	K	3.758	2661	Y	12.704	787	K	3.661	2731
L	6.804	1470	Z	12.925	774	L	3.909	2558	Z	13.130	762	L	3.825	2614
M	7.227	1384	AA	13.877	721	M	6.816	1467	AA	13.250	755	M	4.180	2392
N	7.516	1330				N	7.228	1384	BB	13.362	750	N	4.374	2286
												P	4.916	2034
												Q	6.769	1477
												R	7.244	1380
												S	7.605	1315
												T	8.447	1184
												U	10.006	999
												V	10.736	931
												W	12.461	803
												X	12.565	796
												Y	12.690	788
												Z	13.612	735
												AA	14.730	679

* Probably due to impurity in sodium chloride prism.

For tables of purity of the samples used and for a brief description and statement of the accuracy of the spectrograph used, reference should be made to the preceding paper.

The cell into which the samples were vaporized consists of a stainless steel shell with a concave mirror inside at one end and two sodium chloride windows at the other end. The source is located about 2 cm outside of one window. This provides a separation of the incandescent source from the inflammable octanes. The 2-cm air path does not introduce appreciable absorption due to the carbon dioxide and water vapor in the air. To

eliminate danger of contamination, an all-glass system for filling the cell was devised. The ground glass joints and stopcocks are lubricated with Meloche-Frederick² stopcock lubricant which is composed of glycerin, dextrin, and mannitol. The optical path length of the cell is about 80 cm. The vapor pressures of the octanes at room temperature were sufficiently high that pressures of 15 mm were used in all cases except that of *n*-octane for which a pressure of 12 mm was used.

² C. C. Meloche and W. G. Frederick, J. Am. Chem. Soc. **54**, 3264 (1932).

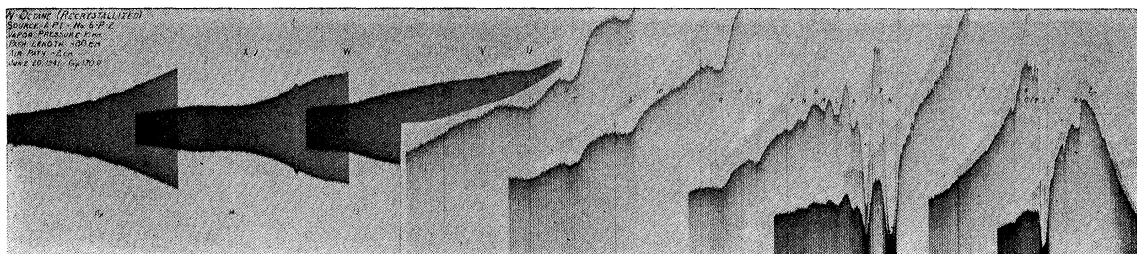


FIG. 1. Infra-red spectrum of *n*-octane.

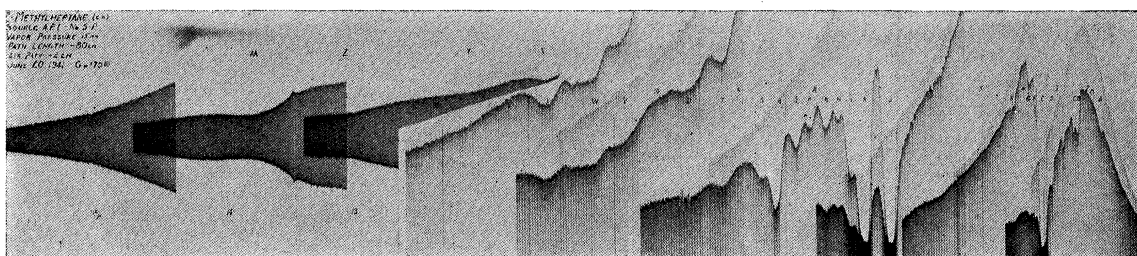


FIG. 2. Infra-red spectrum of 2-methylheptane.

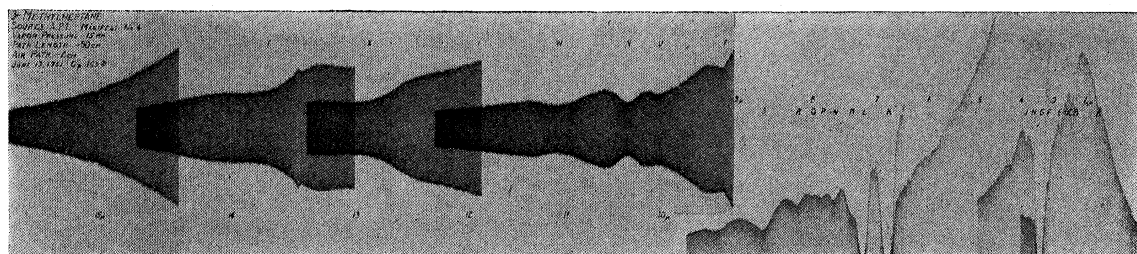


FIG. 3. Infra-red spectrum of 3-methylheptane.

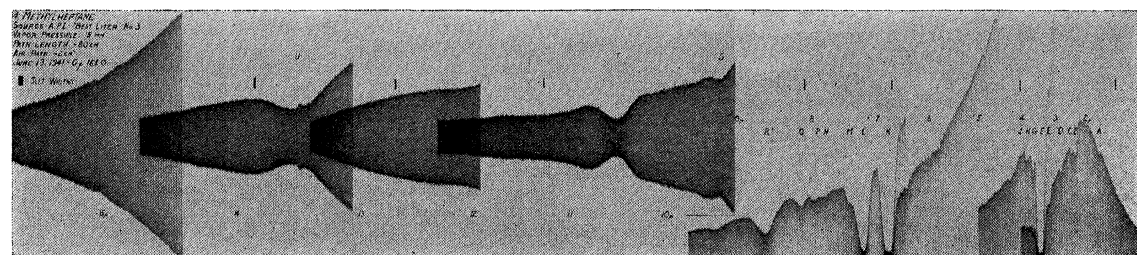


FIG. 4. Infra-red spectrum of 4-methylheptane.

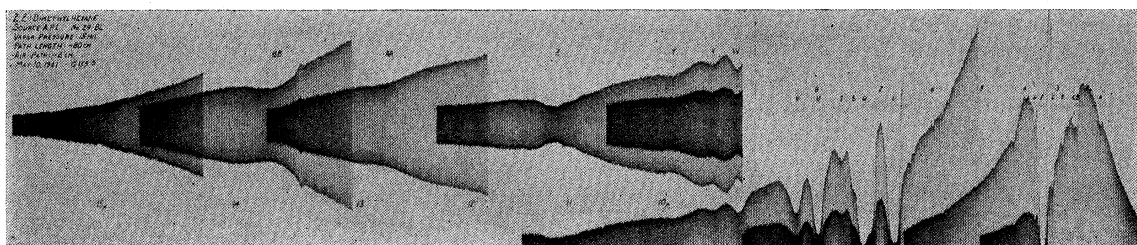


FIG. 5. Infra-red spectrum of 2,2-dimethylhexane

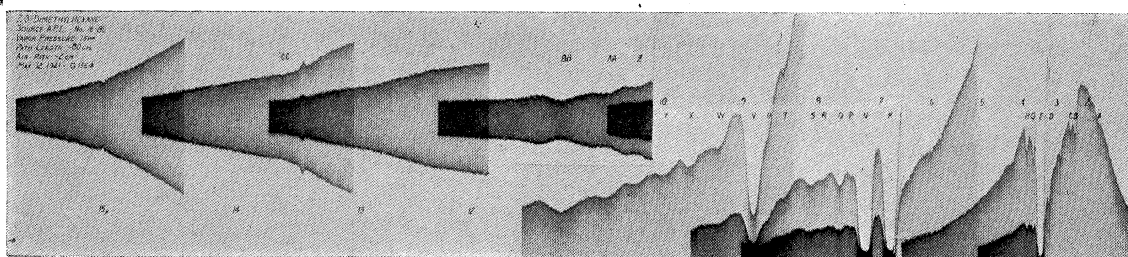


FIG. 6. Infra-red spectrum of 2,3-dimethylhexane.

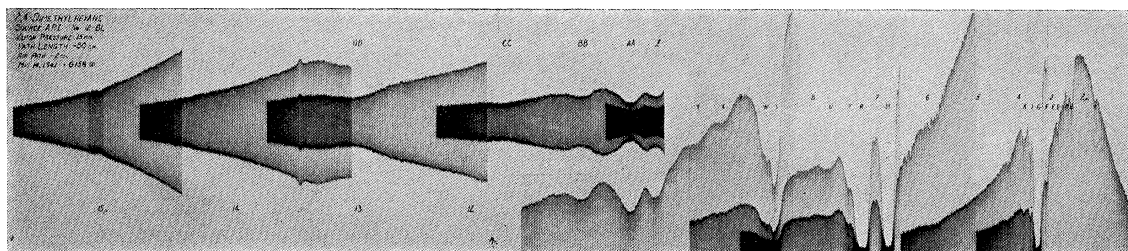


FIG. 7. Infra-red spectrum of 2,4-dimethylhexane.

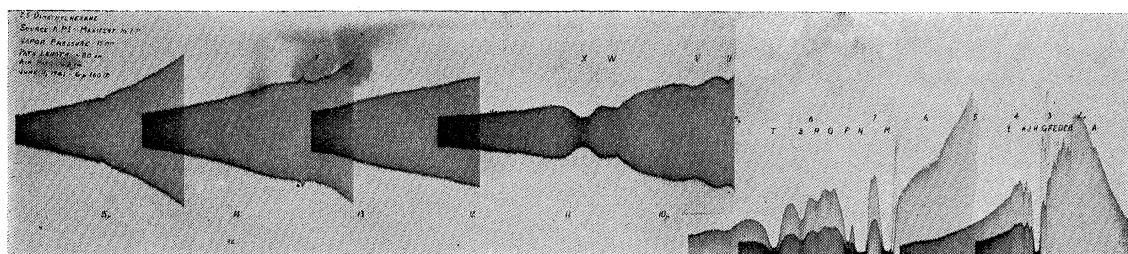


FIG. 8. Infra-red spectrum of 2,5-dimethylhexane.

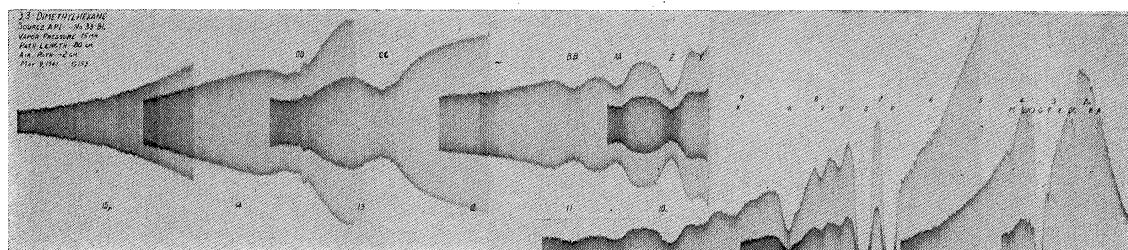


FIG. 9. Infra-red spectrum of 3,3-dimethylhexane.

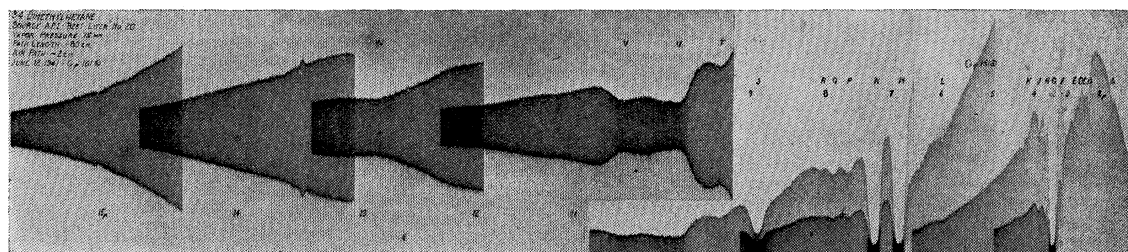


FIG. 10. Infra-red spectrum of 3,4-dimethylhexane.

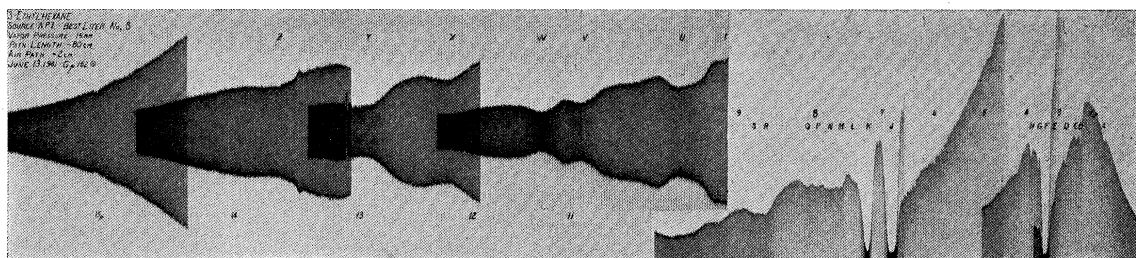


FIG. 11. Infra-red spectrum of 3-ethylhexane.

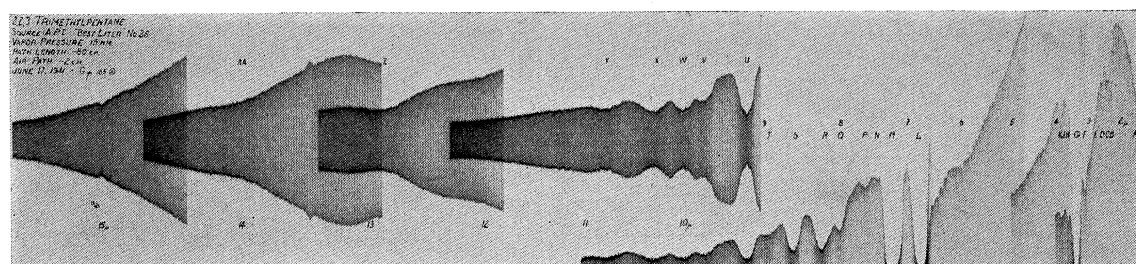


FIG. 12. Infra-red spectrum of 2,2,3-trimethylpentane.

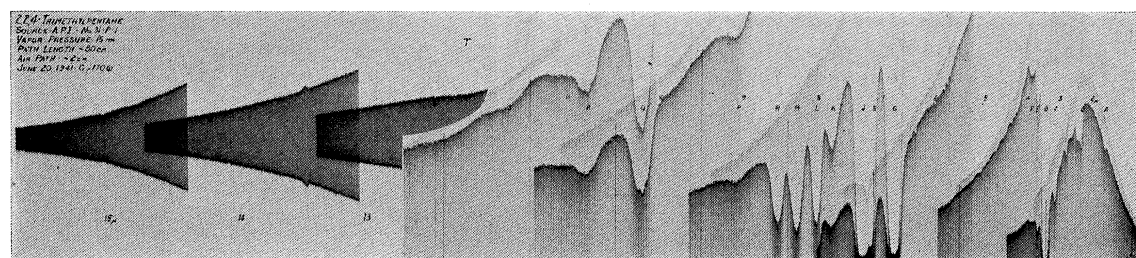


FIG. 13. Infra-red spectrum of 2,2,4-trimethylpentane.

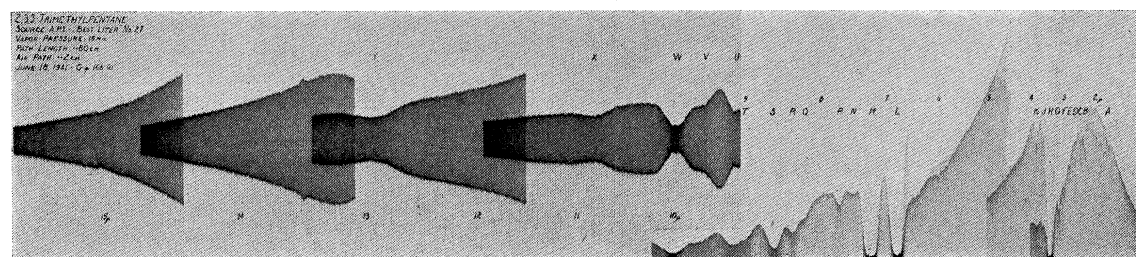


FIG. 14. Infra-red spectrum of 2,3,3-trimethylpentane.

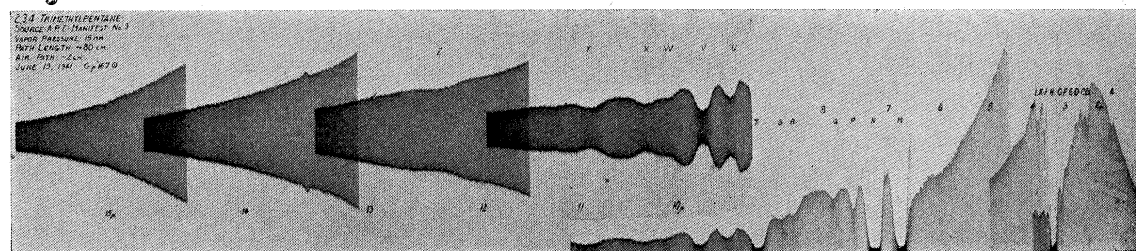


FIG. 15. Infra-red spectrum of 2,3,4-trimethylpentane.

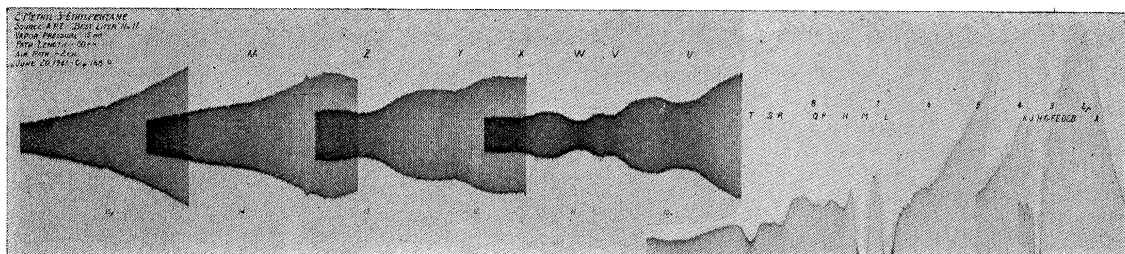


FIG. 16. Infra-red spectrum of 2-methyl, 3-ethylpentane.

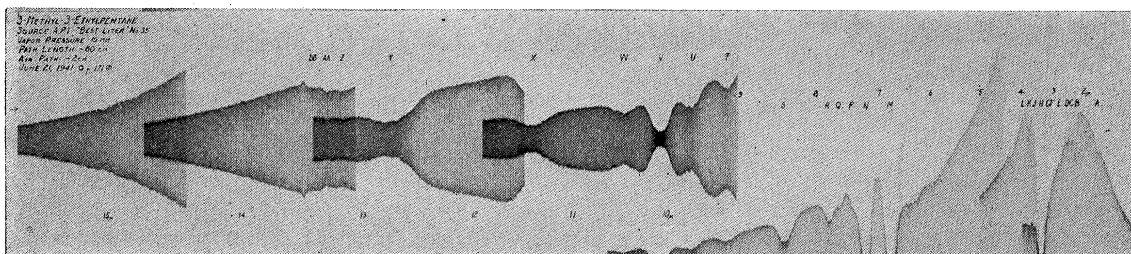


FIG. 17. Infra-red spectrum of 3-methyl, 3-ethylpentane.

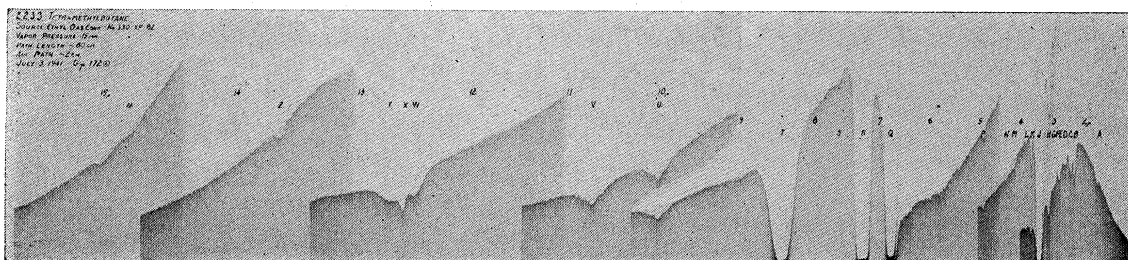


FIG. 18. Infra-red spectrum of 2,2,3,3-tetramethylbutane.

DATA

Figures 1 through 18 are reproductions of the spectra as recorded.

Table I gives the wave-lengths and wave numbers of the absorption lines.

It is not intended to indicate that similarly designated lines in the spectra of different isomers are related. However, lines which bear the same designation in the liquid and vapor phases of the same isomer do have about the same wave-length value.

ACKNOWLEDGMENTS

The hydrocarbons used in this work were prepared under the direction of Professor C. E. Boord 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.

It is again a pleasure to acknowledge the help given by Dr. G. Calingaert and Mr. R. A. Halloran during this investigation.

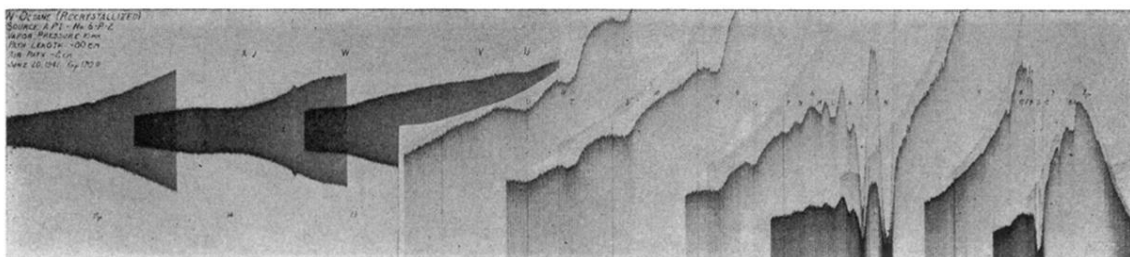


FIG. 1. Infra-red spectrum of *n*-octane.

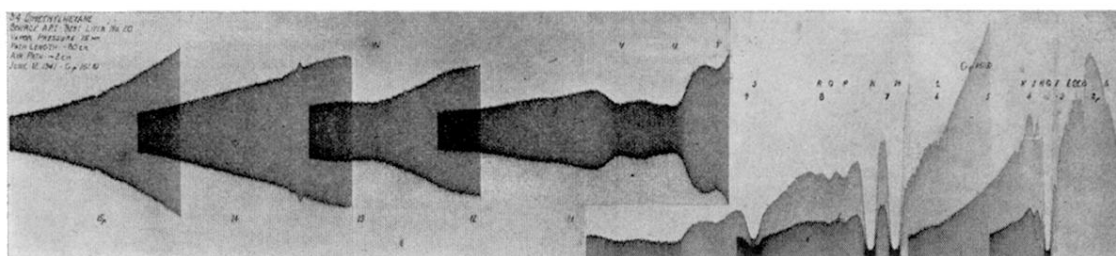


FIG. 10. Infra-red spectrum of 3,4-dimethylhexane.

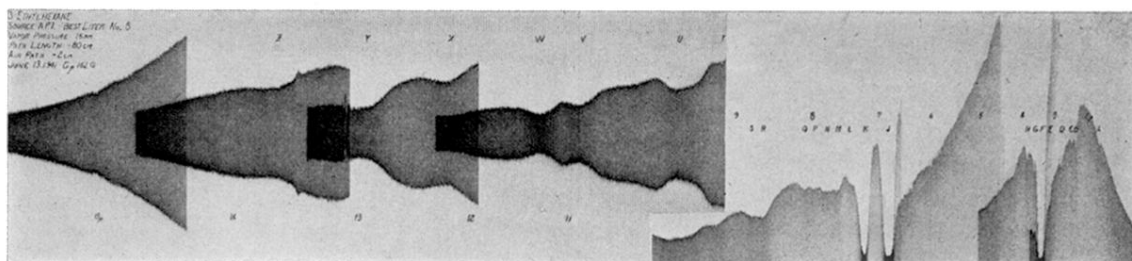


FIG. 11. Infra-red spectrum of 3-ethylhexane.

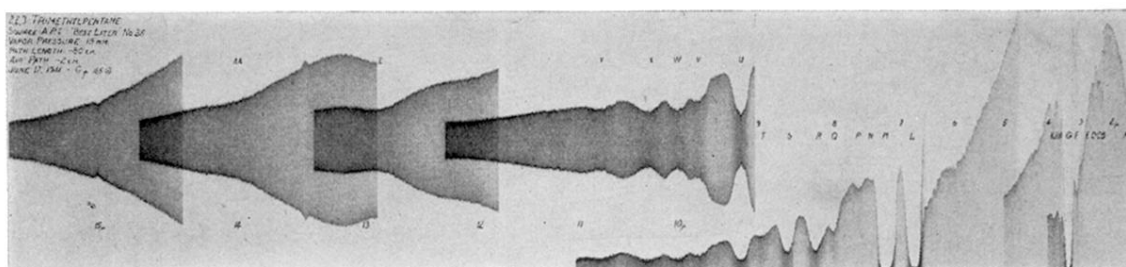


FIG. 12. Infra-red spectrum of 2,2,3-trimethylpentane.

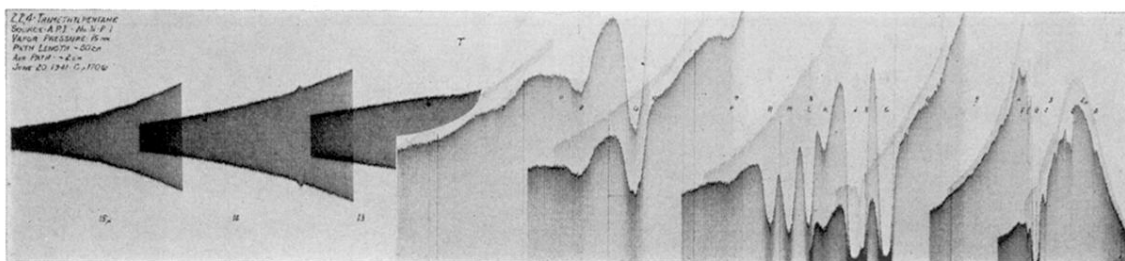


FIG. 13. Infra-red spectrum of 2,2,4-trimethylpentane.

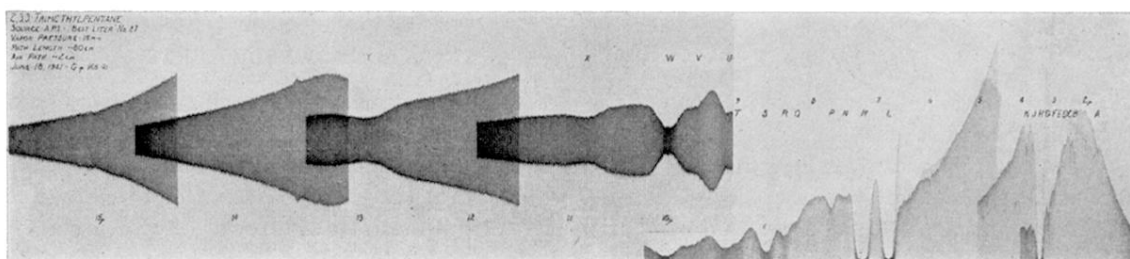


FIG. 14. Infra-red spectrum of 2,3,3-trimethylpentane.

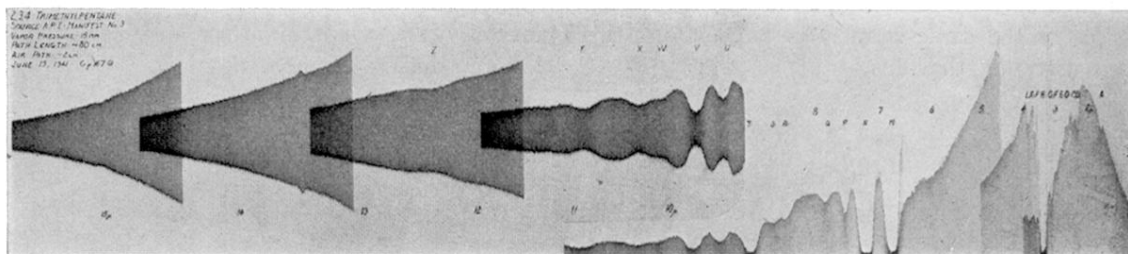


FIG. 15. Infra-red spectrum of 2,3,4-trimethylpentane.

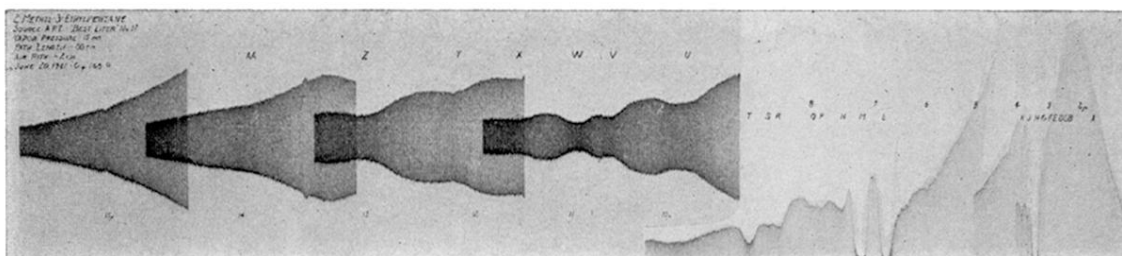


FIG. 16. Infra-red spectrum of 2-methyl, 3-ethylpentane.

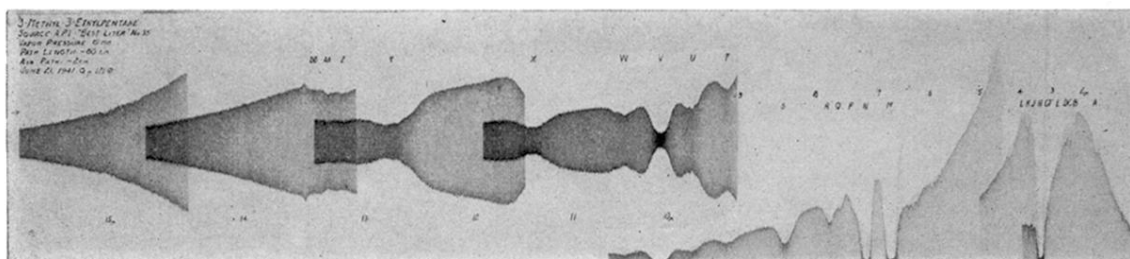


FIG. 17. Infra-red spectrum of 3-methyl, 3-ethylpentane.

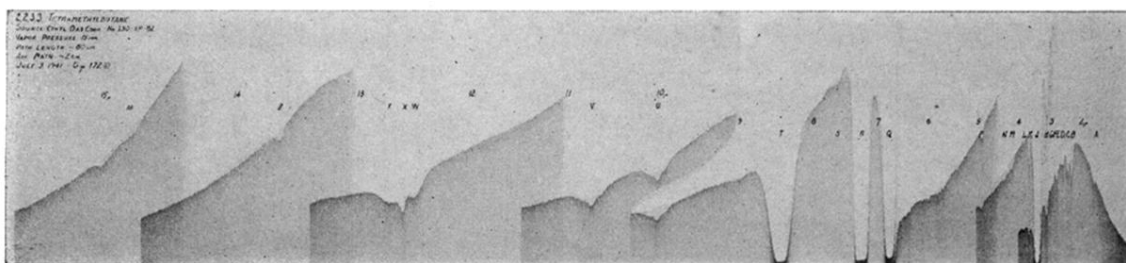


FIG. 18. Infra-red spectrum of 2,2,3,3-tetramethylbutane.

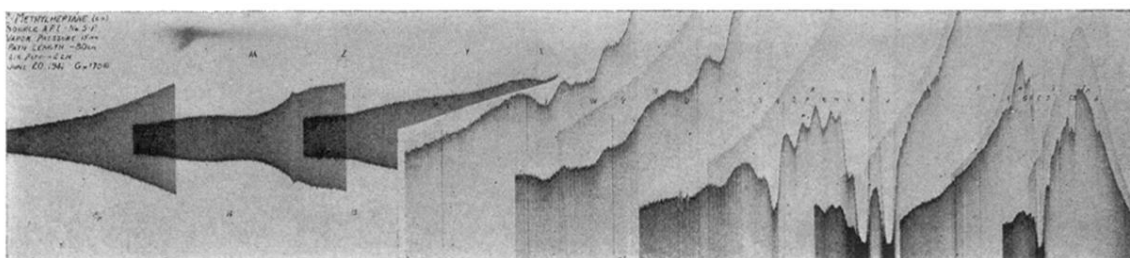


FIG. 2. Infra-red spectrum of 2-methylheptane.

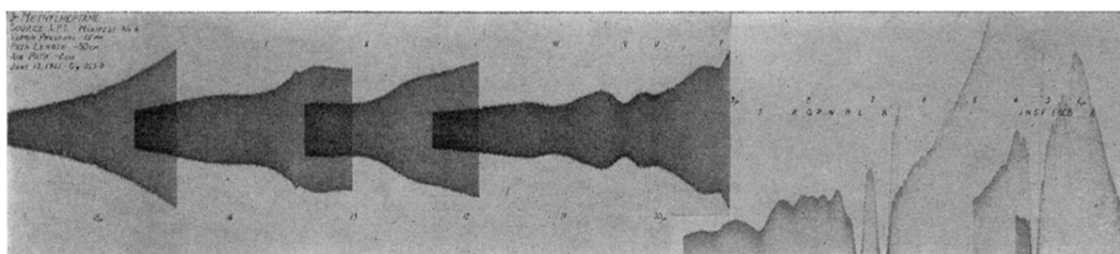


FIG. 3. Infra-red spectrum of 3-methylheptane.

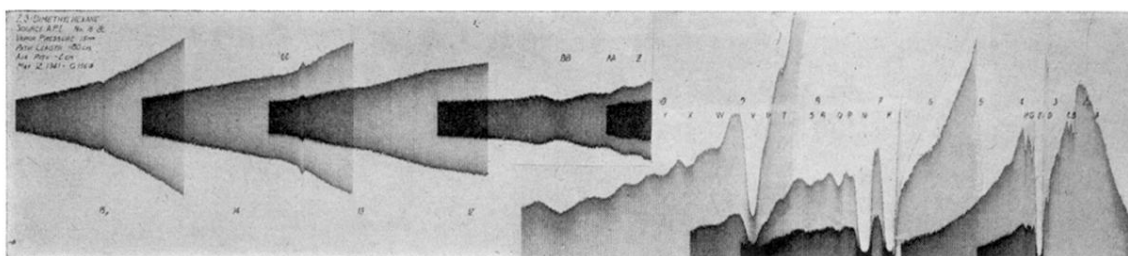


FIG. 6. Infra-red spectrum of 2,3-dimethylhexane.

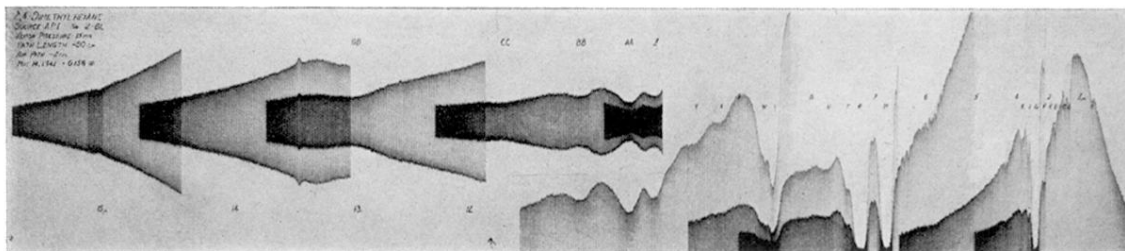


FIG. 7. Infra-red spectrum of 2,4-dimethylhexane.

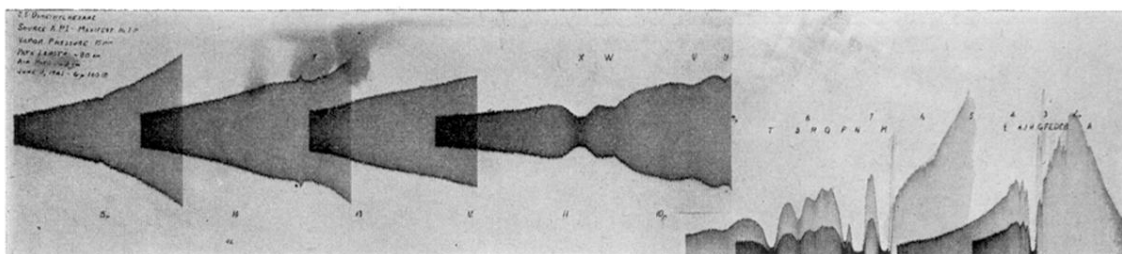


FIG. 8. Infra-red spectrum of 2,5-dimethylhexane.

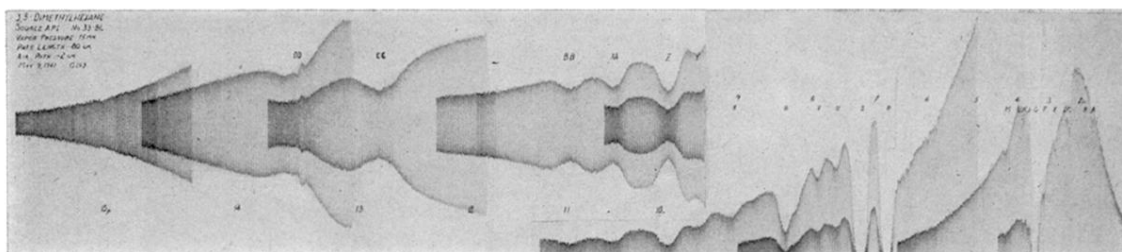


FIG. 9. Infra-red spectrum of 3,3-dimethylhexane.