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Alkylbenzenes in the C_9 Fraction from Seven Representative Crude Petroleums[1] [2]

By Alphonse F. Forziati [3] and Frederick D. Rossini

This report presents the results of an analysis, by analytical distillation by the A. P. I. Research Project 6, and by spectrographic examination by the Socony-Vacuum Laboratories, the Standard Oil Development Co., and the Sun Oil Co. of the individual C_9 alkylbenzenes (except 1,2,3-trimethylbenzene) and of tertbutylbenzene occurring in the C_9 fraction from the following seven representative crudes: (A) Ponca, Okla.; (B) East Texas; (C) Bradford, Pa.; (D) Greendale-Kawkawlin, Mich.; (E) Winkler, Tex.; (F) Midway, Calif.; (G) Conroe, Tex.

I. Introduction

The previous work of the American Petroleum Institute Research Project 6 on the hydrocarbons in the gasoline fraction of seven representative crudes has been described in three earlier reports of investigations [1, 2, 3] *

At the time of the last report, the status of the work was as follows:

(a) Each of the seven naphthas had been separated by adsorption into an aromatic portion and a paraffin-naphthene portion.

(b) Each paraffin-naphthene portion and each aromatic portion had been separately distilled analytically.

(c) For the paraffin-naphthene portion, the analysis of the individual components normally boiling below 102° C had been completed, and, in addition, the amounts of *n*-octane and *n*-nonane had been evaluated. The analysis of the paraffins and naphthenes normally boiling in the range 102° to 180° C was in process.

(d) For the aromatic portion, the analysis of the individual components normally boiling below 160° C has been completed.

Although the eight possible aromatic hydrocarbons whose normal boiling points are below 160° C were relatively easily determined (from measurements of boiling points, refractive indices, and freezing points), the twelve possible aromatic hydrocarbons in the range 160° to 180° C are present in such relatively smaller amounts, and with such small differences in boiling point, that it is possible to obtain from the boiling point-volume curves (on the limited quantity of material processed) only values for close-boiling mixtures (usually pairs). Further, the lack of adequate amounts of nearly pure stocks of each of the component hydrocarbons made it impossible to utilize the method of determining individual hydrocarbons in mixtures of hydrocarbons by measuring freezing points [4,5].

As purified samples of these alkylbenzenes were becoming available for spectrometer calibration, it is was evident that the analysis of the individual aromatic hydrocarbons in the material normally boiling above 160° C could be performed successfully by spectrographic methods. Accordingly, with the approval of the Advisory Committee for the American Petroleum Institute Research Project 6, the cooperation of three laboratories that had experience in the spectrographic analysis of the C_9 alkylbenzenes was enlisted. These laboratories were those of the Socony-Vacuum Oil Co., Paulsboro, N. J., the

[1] This investigation was performed as part of the work of the American Petroleum Institute Research Project 6 on the "Analysis, Purification, and Properties of Hydrocarbons" at the National Bureau of Standards.

[2] Presented before the Division of Petroleum Chemistry of the American Chemical Society at Atlantic City, N. J., April, 1947.

[3] Research Associate on the American Petroleum Institute Research Project 6.

* Figures in brackets indicate the literature references at the end of this paper.

Standard Oil Development Co., Elizabeth, N. J., and the Sun Oil Co., Norwood, Pa. The Socony-Vacuum and Standard Oil Development Laboratories agreed to make infrared and the Sun Oil Laboratory, Raman spectral measurements.

II. Material Analyzed

The seven naphthas under investigation, which have been described in detail in the previous reports [1, 2, 3], are the following: A, Ponca, Okla.; B, East Texas; C, Bradford, Pa.; Greendale-Kawkawlin, Mich.; E, Winkler, Tex.; F, Midway, Calif.; G, Conroe, Tex.

The aromatic portions, boiling between 148° and 180° C, from each of the seven naphthas, were blended,[4] into five lots, as shown in figures 1 to 7, inclusive, which give the temperature-volume curves from the original analytical distillations of these materials, as previously given in the second published report[5] of this work [2].

[4] Although two of the cooperating laboratories preferred to have the blending for spectrographic analysis made from "flat to flat" rather than from "break to break," the material had previously been blended in the latter way for five of the naphthas in order to reduce losses by evaporation and, therefore, the blending for the remaining two naphthas was also made from "break to break." This made the spectrographic analyses more difficult for those laboratories whose normal operating procedures were based on blending from "flat to flat."

[5] The figures 8 to 14 in the previously published report give, except for the Bradford (Pa.) and Winkler (Tex.) naphthas, a plot of refractive index against volume. The aromatic portions of five of the naphthas, Ponca (Okla.), East Texas, Greendale-Kawkawlin (Mich.), Midway (Calif.), and Conroe (Tex.), are seen to be substantially 100 percent aromatic, by comparison of the values of refractive index of the aromatic distillate and of the pure components (indicated by crosses at the appropriate places).

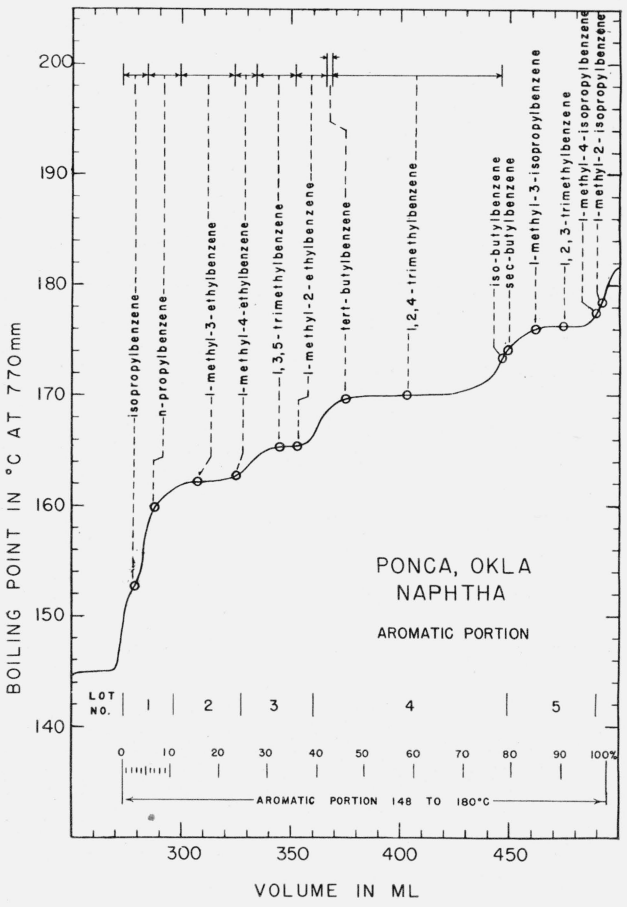

FIGURE 1. *Plot of the boiling point as a function of the volume for the* C_9 *fraction of the aromatic portion of the Ponca, Okla., naphtha.*

The lot numbers refer to the portions of the distillate reblended for spectrographic examination.

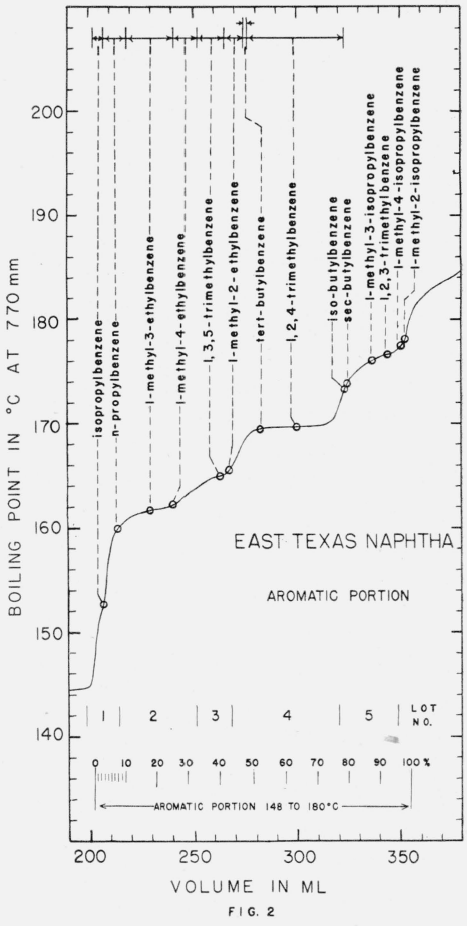

FIG. 2

FIGURE 2. *Plot of the boiling point as a function of the volume for the* C_9 *fraction of the aromatic portion of the East Texas naphtha.*

The lot numbers refer to the portions of the distillate reblended for spectrographic examination.

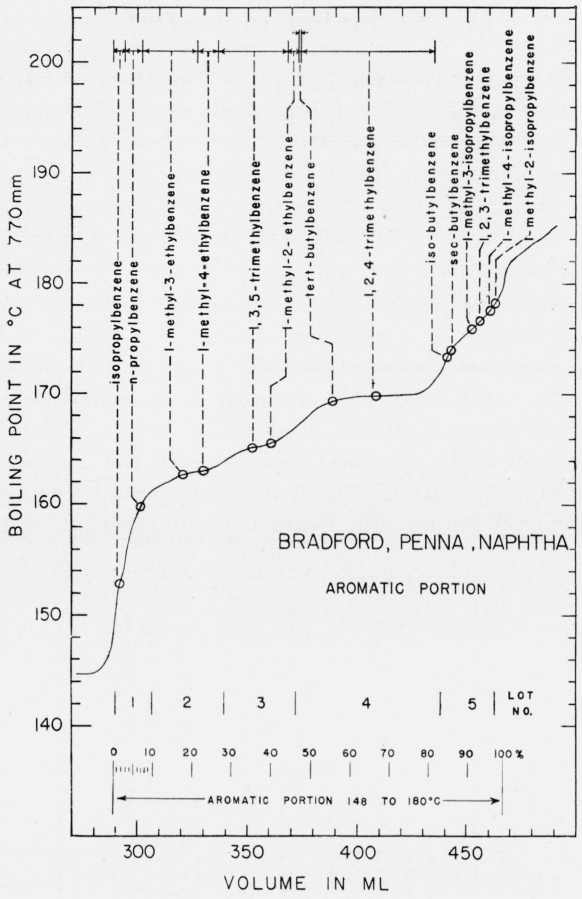

FIGURE 3. *Plot of the boiling point as a function of the volume for the* C_9 *fraction of the aromatic portion of the Bradford, Pa., naphtha.*

The lot numbers refer to the portions of the distillate reblended for spectrographic examination.

At that time, the refractive index-volume plots for the aromatic portion of the Bradford (Pa.) and Winkler (Tex.) naphthas were not shown because the refractive index fell somewhat below the proper values for the aromatic components. Calculations made on the basis of the refractive index expected for 100 percent aromatic material, yielded the following values for the percentage of paraffin-naphthene material remaining in lots 1 to 5:

Bradford (Pa.), naphtha: lot 1, 21 percent; lot 2, 5 percent; lot 3, 5 percent; lot 4, 4 percent; lot 5, 5 percent.

Winkler (Tex.), naphtha: lot 1, 14 percent; lot 2, 3 percent; lot 3, 3 percent; lot 4, 8 percent; lot 5, 14 percent.

For spectrographic examination by the cooperating laboratories, the following samples were prepared and transmitted:

To the Socony-Vacuum Oil Co. and Standard Oil Development Co., for infrared analysis: Samples (4 to 5 ml) of each of the five lots (1 to 5) of each of the seven naphthas.

To the Sun Oil Co., for Raman analysis: Samples (7 to 8 ml) of lot 3 of the East Texas naphtha, and lot 1 of the Bradford, Pa., Greendale-Kawkawlin, Mich., and Midway, Calif., naphthas; Samples (13 to 15 ml) of each of the remaining lots, except lot 1 of East Texas and Conroe, Tex., naphthas.

As the pure hydrocarbons representing the expected components of lot 5 were at that time not yet available for calibrating spectrometers,

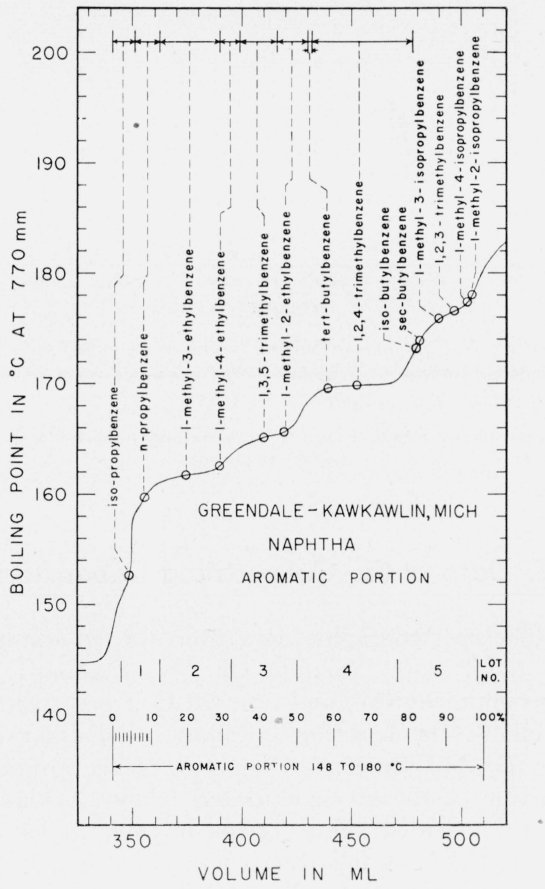

FIGURE 4. *Plot of the boiling point as a function of the volume for the* C_9 *fraction of the aromatic portion of the Greendale-Kawkawlin, Mich., naphtha.*

The lot numbers refer to the portions of the distillate reblended for spectrographic examination.

the cooperating laboratories were requested to report only on lots 1, 2, 3, and 4.

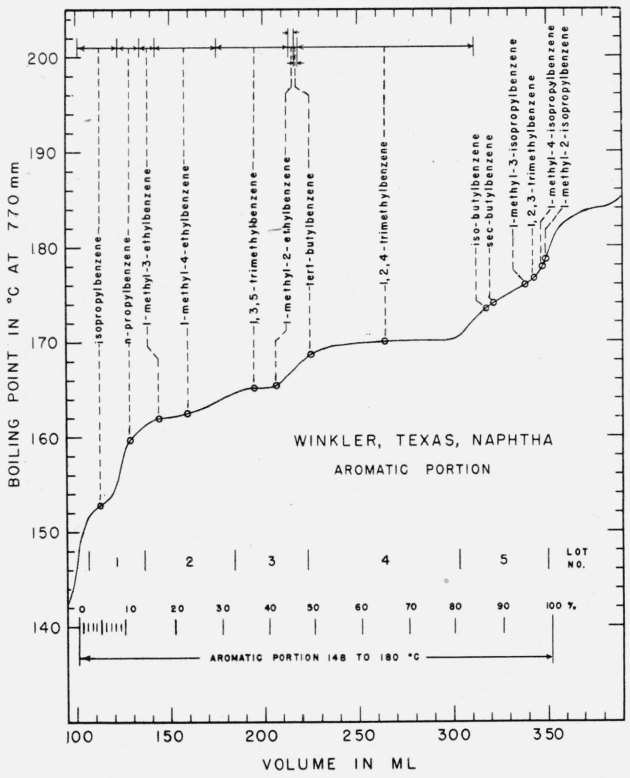

FIGURE 5. *Plot of the boiling point as a function of the volume for the* C_9 *fraction of the aromatic portion of the Winkler, Tex., naphtha.*

The lot numbers refer to the portions of the distillate reblended for spectrographic examination.

III. Data of the Cooperating Laboratories

The spectrographic data from the laboratories of the Socony Vacuum Oil Co., Standard Oil Development Co., and Sun Oil Co., are given in table 1. The data from the analytical distillations, by the API Research Project 6, of the aromatic portion of the seven naphthas (shown in figures 1 to 7) yielded values (given in table 2) for the amounts of the following components or pairs of components: isopropylbenzene; *n*-propylbenzene; 1-methyl-3-ethylbenzene plus 1-methyl-4-ethylbenzene; 1,3,5-trimethylbenzene plus 1-methyl-2-ethylbenzene; tert-butylbenzene plus 1,2,4-trimethylbenzene.

IV. Evaluation of the Data

From the values reported by the three laboratories on the spectrographic analysis of the several lots of the seven naphthas, the total amount of each component found by a given laboratory in all four lots (1 to 4) was computed. These values, given for each component for each naphtha analyzed, and expressed as a percentage by volume of the aromatic portion 148° to 180° C, are given in columns 2, 3, and 4 of table 2. In the case of the East Texas, Bradford (Pa.), and Conroe (Tex.) naphthas, the values for 1-methyl-3-ethylbenzene from the Sun Oil Co. were increased as shown, the increase being simply the average of the amounts of this component found by the Socony-Vacuum and Standard Oil Development

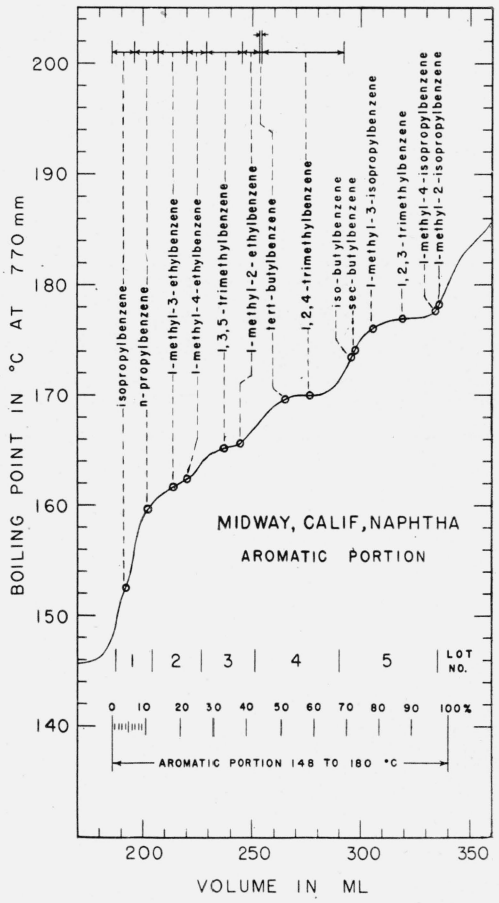

FIGURE 6. *Plot of the boiling point as a function of the volume for the* C_9 *fraction of the aromatic portion of the Midway, Calif., naphtha.*

The lot numbers refer to the portions of the distillate reblended for spectrographic examination.

TABLE 1. *The amounts of the individual hydrocarbons in lots 1 to 4 of the C_9 aromatic portion of the seven representative naphthas, as determined spectrographically by the three laboratories*

Lot number and hydrocarbons	Naphtha (see text)																			
	A			B			C			D			E			F			G		
	Laboratory[b]																			
	I	II	III	I	II	III	I	II	III	I	II	III	I	II	III	I	II	III	I	II	III
	Percentage by volume of the given lot																			
Lot 1																				
o-xylene	3	9	12	3	14	–	3	13	–	3	8	9.5	0	2	0	6	18	16.5	6	16	–
isopropylbenzene	27	42	25	27	41	–	12	18	–	12	29	14	49	62	55.5	38	51	39.5	14	23	–
n-propylbenzene	60	45	48.5	59	34	–	47	18	–	57	41	44	45	14	18	50	28	33	45	32	–
1-methyl-3-ethylbenzene	10	2	14.5	11	8	–	38	13	–	28	17	27.5	4	7	11.5	6	0	11	35	23	–
1-methyl-4-ethylbenzene	0	2	0	0	3	–	0	4	–	0	5	5	2	15	15	0	3	0	0	6	–
Lot 2																				
isopropylbenzene	0	1	–	0	0	–	0	0	–	0	3	–	0	0	–	0	2	–	0	0	–
n-propylbenzene	16	10	13	16	10	10.5	12	3	9.5	16	9	10.5	14	0	–	21	25	–	15	8	7
1-methyl-3-ethylbenzene	67.7	62	64.5	56	54	56	61	44	54	64	54	66	15	10	–	54	35	–	60	55	64.5
1-methyl-4-ethylbenzene	16	22	21.5	19	26	26.5	15	19	20.5	16	22	20	55	60	–	18	22	–	15	23	18
1,3,5-trimethylbenzene	0.3	3	1	6	6	7	10	17	16	3	3	3.5	15	21	–	5	8	–	8	11	10.5
1-methyl-2-ethylbenzene	0	2	0	3	4	0	2	3	0	1	0	0	1	1	–	2	1	–	2	3	0
tert-butylbenzene	–	0	–	–	0	–	–	0	–	–	0	–	–	1	–	–	0	–	–	0	–
1,2,4-trimethylbenzene	–	0	–	–	0	–	–	0	–	–	0	–	–	7	–	–	0	–	–	0	–
Lot 3																				
1-methyl-3-ethylbenzene	9	11	8	9	9	9.5	5	8	7	9	11	8	0	1	–	11	10	10	5	4	7.5
1-methyl-4-ethylbenzene	8	9	9.5	8	8	9.5	3	7	9.5	8	9	11.5	2	8	–	12	13	15.5	3	6	6
1,3,5-trimethylbenzene	46	41	42.5	50	45	41.5	71	65	65	49	41	40	78	64	–	49	39	36.5	60	45	49
1-methyl-2-ethylbenzene	28	30	33	27	33	37.5	9	12	12.5	28	33	37.5	4	8	–	21	28	32.5	10	17	11.5
tert-butylbenzene	0	4	0	0	3	0	0	1	0	0	3	0	0	3	–	0	4	0	0	3	0
1,2,4-trimethylbenzene	9	5	7	6	2	2	12	7	6	6	3	3	16	16	–	7	6	5.5	22	25	26
Lot 4																				
1-methyl-4-ethylbenzene	–	0	–	–	0	–	–	0	–	–	0	–	–	0	–	–	4	–	–	0	–
1,3,5-trimethylbenzene	4	5	2.5	6	5	5	10	11	8	5	6	4	4	5	–	9	9	5	2	0	1
1-methyl-2-ethylbenzene	3	8	5.5	4	9	5	2	2	0	4	9	7	0.5	2	–	4	6	6.5	0.5	2	0
tert-butylbenzene	0.7	1	2.5	0.5	1	3	0	1	0	0	2	2.5	1	1	–	0.7	1	0	0.5	2	2
1,2,4-trimethylbenzene	83.5	76	88.5	85	74	86	83.2	72	92	90	71	86.5	93.5	74	–	83.5	69	97	90.7	77	96
Iso-butylbenzene	0	a	0	0	a	0	0	a	0	0	a	0	0	a	–	0	a	0	0	a	0
1,2,3-trimethylbenzene	0.8	a	1	0.5	a	1	0.8	a	0	0	a	0	0	a	–	0.8	a	1.5	0.8	a	1

[a] Values determined but not reported.

[b] The Roman numerals identify the following laboratories and methods used: I, Socony-Vacuum Oil Co., infrared; II, Standard Oil Development Co., infrared; III, Sun Oil Co., Raman.

TABLE 2. *Results of the analyses of the C_9 alkylbenzenes (except 1,2,3-trimethylbenzene) and tert-butylbenzene in the seven naphthas*

Hydrocarbon	Analysis																															
	By Socony-Vacuum							By Standard Oil Dev.							By Sun Oil							By A.P.I. RP 6							Average Value						
	A	B	C	D	E	F	G	A	B	C	D	E	F	G	A	B	C	D	E	F	G	A	B	C	D	E	F	G	A	B	C	D	E	F	G
	Percentage by volume of the aromatic portion, 148° to 180° C.																																		
isopropylbenzene	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	5.0	3.3	2.8	5.9	8.4	6.5	4.0	5.0	3.3	2.8	5.9	8.4	6.5	4.0
n-propylbenzene	8.4	10.0	6.5	8.9	8.1	8.3	6.9	6.1	6.0	2.2	5.9	1.7	6.6	4.2	6.8	–	–	6.5	–	–	–	5.0	6.5	5.6	5.3	4.8	6.5	5.3	6.6	7.5	4.8	6.6	4.9	7.1	5.5
1-methyl-3-ethylbenzene	11.8	15.7	15.7	17.0	3.4	10.3	18.1	10.5	14.7	10.8	14.3	2.9	6.7	16.0	11.7	15.6[b]	13.7[b]	17.2	–	–	19.3[b]														
1-methyl-4-ethylbenzene	3.4	5.5	3.4	4.6	11.1	4.5	4.3	4.6	7.5	5.2	6.4	14.5	6.6	7.4	4.4	7.5	5.6	6.5	–	–	5.8	17.6	20.9	20.8	23.1	16.5	14.3	22.5	15.6 / 4.3	21.8 / 6.8	18.8 / 5.0	22.3 / 5.9	16.1 / 12.9	14.1 / 5.6	23.4 / 5.8
1,3,5-trimethylbenzene	8.5	9.1	18.8	10.7	16.3	10.6	17.5	8.5	8.2	19.3	9.6	15.6	9.5	14.0	7.5	8.0	18.0	8.9	–	–	15.1														
1-methyl-2-ethylbenzene	5.4	5.1	2.8	6.3	1.0	4.6	3.1	7.9	7.8	3.5	8.4	2.1	6.0	5.5	7.1	5.9	2.3	8.6	–	–	2.9	13.6	15.0	18.0	17.7	16.1	17.5	21.2	14.6 / 6.6	14.8 / 6.3	20.7 / 2.7	17.6 / 7.8	17.0 / 1.5	16.1 / 5.6	19.8 / 3.8
tert-butylbenzene	0.3	0.2	0	0	0.3	0.2	0.1	1.0	0.7	0.6	1.1	1.0	0.9	1.3	1.0	1.0	0	0.7	–	–	0.5														
1,2,4-trimethylbenzene	36.0[a]	32.3[a]	35.9[a]	30.4[a]	39.5[a]	25.8[a]	30.7[a]	32.4[a]	28.1[a]	30.3[a]	24.7[a]	34.6[a]	22.0[a]	27.9[a]	37.7[a]	32.2[a]	37.5[a]	28.9[a]	–	–	33.1[a]	35.8	32.0	35.4	29.0	38.1	24.7	31.1	36.0 / 35.2	31.6 / 31.0	34.9 / 34.7	28.7 / 28.1	37.8 / 37.2	25.0 / 24.5	31.2 / 30.6

[a] The observed value has been increased to allow for the amount of 1,2,4 trimethylbenzene estimated to be in lot 5 (the analysis of which was not reported), as follows: A, 1.2 percent; B, 2.2 percent; C, 2.2 percent; D, 4.7 percent; E, 7.2 percent; F, 3.7 percent; G, 1.7 percent.

[b] The observed value has been increased to allow for the amount of 1-methyl-3-ethylbenzene estimated to be in lot 1 (the analysis of which was not reported as follows: B, 1.0 percent; C, 2.3 percent; G, 2.1 percent.

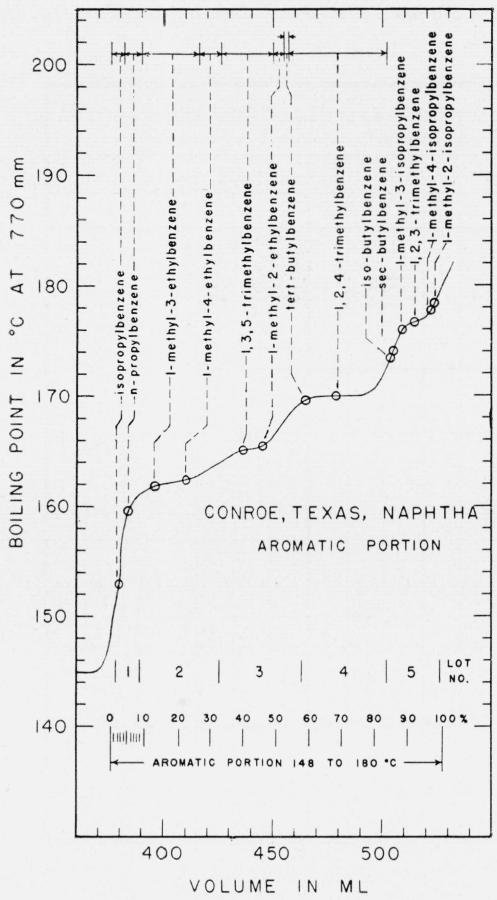

FIGURE 7. *Plot of the boiling point as a function of the volume for the* C_9 *fraction of the aromatic portion of the Conroe, Tex., naphtha.*

The lot numbers refer to the portions of the distillate reblended for spectrographic examination.

laboratories in lot 1, which, for these naphthas, was not analyzed by the Sun Oil laboratory. Uniformly for the spectrographic values from all three laboratories, the amount of 1,2,4-trimethylbenzene was increased by the amount indicated, in order to account for the amount of this component expected to be in lot 5, which has not yet been analyzed spectrographically. The amount to be added was deduced from a correlation of the value for the amount of tert-butylbenzene plus 1,2,4-trimethylbenzene reported by the API Research Project 6, which includes the amount of this component in lot 5, with the boiling point at the end of lot 4, for each naphtha. This correction to the amount of 1,2,4-trimethylbenzene is smallest (1.2%) for the Ponca (Okla.) naphtha and largest (7.2%) for the Winkler (Tex.) naphtha, which is in accord with the fact that the boiling point at the end of lot 4 is highest for the Ponca (Okla.) naphtha and lowest for the Winkler (Tex.) naphtha.

The values from the boiling point-volume data of the API Research Project 6 are given in column 5 of table 2.

The values given in the last column of table 2, representing the final selected "best" values for the amount of each of the given components in each naphtha, were obtained in the following way:

(a) The amount of isopropylbenzene was taken to be that given by the data of the API Research Project 6. (A more accurate value for isopropylbenzene could have been obtained from the spectrographic data if the material just preceding lot 1 could have been examined spectrographically, so that spectrographic values for the total amount of this component would have been available.)

(b) The amount of *n*-propylbenzene was taken as the average of the values from the four (or three) laboratories, as given.

(c) The sum of the amounts of 1-methyl-3-ethylbenzene and 1-methyl-4-ethylbenzene was taken as the average of the values from the four (or three) laboratories, as given. The relative amounts of the two components was taken as the average of the relative amounts given by the spectrographic analyses.

(d) The final values for 1,3,5-trimethylbenzene and 1-methyl-2-ethylbenzene were obtained in a manner exactly analogous to the procedure described for 1-methyl-3-ethylbenzene and 1-methyl-4-ethylbenzene.

(e) The final values for tert-butylbenzene and 1,2,4-trimethylbenzene were obtained in the same manner as the preceding pair.

V. Summary of the Results

Table 3 gives, for the seven naphthas, the amounts of the C_9 alkylbenzenes (except 1,2,3-trimethylbenzene) and tert-butylbenzene, expressed as a percentage by volume of (a) the total aromatics to 180° C; (b) the naphtha 40° to 180° C; (c) the crude petroleum.

Table 4 gives the relative amounts of the C_9 alkylbenzenes (except 1,2,3-trimethylbenzene) and tert-butylbenzene in the seven representative naphthas.

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TABLE 3. *Summary of the amounts of the C_9 alkylbenzenes (except 1,2,3-trimethylbenzene) and tert-butylbenzene in the seven naphthas*

Hydrocarbon	Amount of the given hydrocarbon expressed as percentage by volume of																				
	Total aromatics to 180°C.							Naphtha 40° to 180°C.							Crude Petroleum						
	A	B	C	D	E	F	G	A	B	C	D	E	F	G	A	B	C	D	E	F	G
isopropylbenzene	2.2	1.4	1.1	2.0	6.0	3.0	1.2	0.22	0.12	0.11	0.13	0.22	0.19	0.33	0.07	0.04	0.03	0.03	0.03	0.03	0.09
n-propylbenzene	3.0	3.2	1.8	2.2	3.5	3.2	1.6	0.29	0.28	0.18	0.15	0.13	0.21	0.46	0.09	0.08	0.05	0.03	0.02	0.04	0.12
1-methyl-3-ethylbenzene	5.2	6.5	5.2	5.4	2.3	3.9	5.0	0.51	0.57	0.52	0.37	0.08	0.25	1.47	0.17	0.16	0.13	0.08	0.01	0.04	0.40
1-methyl-4-ethylbenzene	1.9	2.9	1.9	1.9	9.2	2.6	1.7	0.19	0.26	0.19	0.13	0.34	0.17	0.49	0.06	0.07	0.05	0.03	0.05	0.03	0.13
1,3,5-trimethylbenzene	3.6	3.7	6.8	3.2	11.0	4.8	4.6	0.35	0.32	0.68	0.22	0.40	0.31	1.34	0.12	0.09	0.17	0.05	0.05	0.05	0.36
1-methyl-2-ethylbenzene	3.0	2.7	1.0	2.6	1.1	2.6	1.1	0.29	0.24	0.10	0.18	0.04	0.17	0.32	0.09	0.07	0.03	0.04	0.01	0.03	0.09
tert-butylbenzene	0.4	0.3	0.1	0.2	0.4	0.2	0.2	0.03	0.02	0.01	0.01	0.02	0.02	0.05	0.01	0.01	0.00_2	0.00_3	0.00_2	0.00	0.01
1,2,4-trimethylbenzene	15.8	13.4	13.2	9.3	26.5	11.2	8.8	1.53	1.18	1.31	0.64	0.97	0.72	2.56	0.51	0.34	0.33	0.15	0.13	0.13	0.69

TABLE 4. *Relative amounts of the C_9 alkylbenzenes (except 1,2,3-trimethylbenzene) and tert-butylbenzene in seven representative naphthas*

Compound	Naphtha (See text)							Range of values	Average value
	A	B	C	D	E	F	G		
	Relative amounts								
Isopropylbenzene	6.4	4.2	3.4	7.3	10.0	9.5	4.8	3 to 10	7
n-Propylbenzene	8.4	9.5	5.9	8.1	5.8	10.3	6.5	6 to 10	8
1-Methyl-3-ethylbenzene	15.0	19.0	16.8	20.2	3.8	12.4	21.0	[a] 4 to 21	15
1-Methyl-4-ethylbenzene	5.5	8.6	6.1	7.3	15.3	8.1	6.9	6 to [b] 15	8
1,3,5-Trimethylbenzene	10.2	10.7	22.0	12.1	18.4	15.3	19.1	10 to 22	15
1-Methyl-2-ethylbenzene	8.5	8.0	3.3	9.6	1.8	8.1	4.5	2 to 10	6
tert-Butylbenzene	1.0	0.8	0.2	0.7	0.7	0.7	0.7	0 to 1	1
1,2,4-Trimethylbenzene	45.0	39.2	42.3	34.7	44.2	35.6	36.5	35 to 45	40
Total	100	100	100	100	100	100	100	-------	100

[a] Excluding naphtha E, the lower limit here would be 12 instead of 4.
[b] Excluding naphtha E, the upper limit here would be 9 instead of 15.

The results of the present investigation indicate that the alkylbenzenes in the C_9 fraction of petroleum are present in relative amounts that are of the same magnitude for different crude petroleums, with the exception that in the Winkler, Tex., naphtha, E, the 1-methyl-3-ethylbenzene and the 1-methyl-4-ethylbenzene are reversed from the usual order. The range and average values are given in the last column of table 4. This follows similar relations previously reported for the lower alkylbenzenes and for certain other groups of hydrocarbons in different crudes.

Although the connection is not apparent at this writing the average relative amounts of the five polyalkylbenzenes listed in table 4, representing the average relative occurrence of these compounds in the liquid state in these petroleums, are remarkably close to the relative amounts of these five compounds that would be present at thermodynamic equilibrium in the gas phase at 400°C as calculated from recently published thermodynamic

data for these compounds [6]. The relative amounts of these five polyalkylbenzenes are as follows, for the liquid state in these natural petroleums, on the average, and for thermodynamic equilibrium in the gas phase at 400°C, respectively: 1-methyl-2-ethylbenzene, 7, 6; 1-methyl-3-ethylbenzene, 18, 17; 1-methyl-4-ethylbenzene, 9, 11; 1,2,4-trimethylbenzene; 48, 48; 1,3,5-trimethylbenzene, 18, 18. The relative amounts of the two propylbenzenes do not, however, show any accord with the foregoing.

Information regarding the spectrographic apparatus and procedure used by the laboratories of the Socony-Vacuum Oil Co., the Standard Oil Development Co., and the Sun Oil Co. in the spectrographic analyses reported here may be obtained directly from those laboratories.

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