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The Refractive Indices and Densities of Ternary Mixtures of Benzene–Toluene–Xylene

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The relationship between the composition of the ternary mixtures of benzene–toluene–xylene and the refractive index, as well as density, was determined at 25 °C.

Relationships between the composition and refractive index, as well as density, are known in literature for the binary mixtures: benzene–toluene, benzene–xylene, and toluene–xylene (*6*). With the aim to use ternary mixtures of benzene–toluene–xylene as the test mixture for distillation columns, the examination of the relationship between composition and density along with index of refraction was undertaken.

Experimental Section

For preparation of different solutions of the ternary mixture, reagent grade pro analysis (Merck) was used, with the following data:

	Bp at 760 mmHg t, °C	Density $d^{25\,°\mathrm{C}}_{4}$ g ml^{-1}	RI $n^{25°\mathrm{C}}_{\mathrm{D}}$
Benzene	80.1	0.8779	1.497 10
Toluene	110.6	0.8649	1.493 66
Xylene	138.5	0.8639	1.494 90

This is in good agreement with the data reported in literature (*4*, *6*). The density and refractive index mean deviations are 0.6 and 0.05%, respectively.

The solutions were prepared by weight, the binary mixture benzene–toluene being prepared first in 20 mol % intervals with subsequent addition of xylene. Required precautions were applied to prevent any loss due to evaporation. Individual component weights were determined by a Mettler balance Type H20 with an accuracy of ±0.005%.

Densities and the refractive index of prepared solutions were determined in duplicate at 25 °C. The temperature was controlled within ±0.005 °C by an Ultra-Thermostat. A Zeiss refractometer was used to observe the refractive index with an accuracy of ±0.005%. For the determination of densities Ostwald's pycnometers were used.

Table I. Benzene–Toluene System

Benzene composition, mole fraction	Density, $d^{25°\mathrm{C}}_{4}$, g ml^{-1}	Refractive index (±0.000 05), $n^{25°\mathrm{C}}_{\mathrm{D}}$
0.00	0.8649	1.493 66
0.20	0.8675	1.494 15
0.40	0.8705	1.494 95
0.60	0.8734	1.495 60
0.80	0.8760	1.496 35
1.00	0.8779	1.497 10

Table II. Benzene–Xylene System

Benzene composition, mole fraction	Density, $d^{25°\mathrm{C}}_{4}$, g ml^{-1}	Refractive index (±0.000 05), $n^{25°\mathrm{C}}_{\mathrm{D}}$
0.00	0.8639	1.494 90
0.20	0.8645	1.494 85
0.40	0.8670	1.495 00
0.60	0.8700	1.495 30
0.80	0.8737	1.496 00
1.00	0.8779	1.497 10

Table III. Toluene–Xylene System

Toluene composition, mole fraction	Density, $d^{25°\mathrm{C}}_{4}$, g ml^{-1}	Refractive index (±0.000 05), $n^{25°\mathrm{C}}_{\mathrm{D}}$
0.00	0.8639	1.494 90
0.20	0.8642	1.494 70
0.40	0.8645	1.494 50
0.60	0.8646	1.494 20
0.80	0.8648	1.493 90
1.00	0.8649	1.493 66

Results

The obtained results are presented in Tables I–IV. The density–composition and refractive index–composition curves are shown on Figures 1–3.

Table IV. Benzene–Toluene–Xylene System

Relation of benzene to toluene mole fractions	Benzene composition, mole fraction	Toluene composition, mole fraction	Xylene composition, mole fraction	Density $d^{25°C}{}_4$, g ml^{-1}	Refractive index (±0.000 05), $n^{25°C}{}_D$
0.250	0.20	0.80	0.00	0.8675	1.494 15
0.250	0.16	0.64	0.20	0.8673	1.494 00
0.250	0.12	0.48	0.40	0.8671	1.494 05
0.250	0.08	0.32	0.60	0.8666	1.494 20
0.250	0.04	0.16	0.80	0.8660	1.494 45
0.666	0.40	0.60	0.00	0.8705	1.494 95
0.666	0.32	0.48	0.20	0.8702	1.494 58
0.666	0.24	0.36	0.40	0.8694	1.494 48
0.666	0.16	0.24	0.60	0.8683	1.495 00
0.666	0.08	0.12	0.80	0.8668	1.496 00
1.500	0.60	0.40	0.00	0.8734	1.495 60
1.500	0.48	0.32	0.20	0.8723	1.495 00
1.500	0.36	0.24	0.40	0.8714	1.494 70
1.500	0.24	0.16	0.60	0.8700	1.494 65
1.500	0.12	0.08	0.80	0.8678	1.494 68
4.000	0.80	0.20	0.00	0.8760	1.496 35
4.000	0.64	0.16	0.20	0.8751	1.495 30
4.000	0.48	0.12	0.40	0.8737	1.494 92
4.000	0.32	0.08	0.60	0.8720	1.494 71
4.000	0.16	0.04	0.80	0.8687	1.494 75

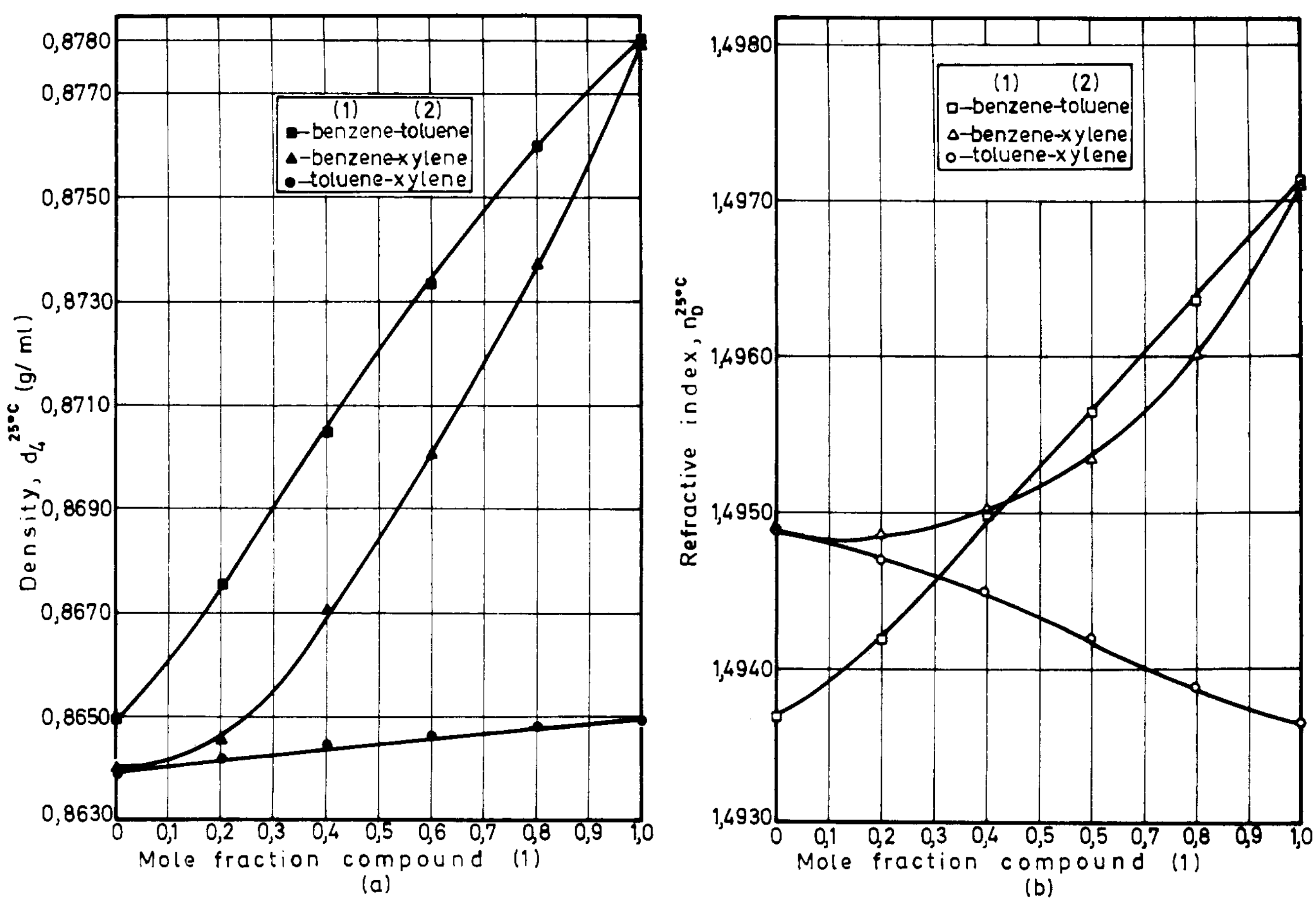

Figure 1. Densities (a) and refractive indices (b) of benzene–toluene, benzene–xylene, and toluene–xylene systems at 25 ± 0.005 °C.

The data for the curves on diagram 3 were derived from the curves of diagrams 1 and 2.

Discussion

The IBM 1130 computer was used for mathematical processing of experimental data. The results were correlated by use of the method of least squares.

The relationships for density–composition and refractive index–composition are presented by eq 1–8:

Benzene–Toluene System:

$$d^{25\,°C}{}_4 = 0.8649 + 0.0117x_1 + 0.0083x_1^2 - 0.0071x_1^3 \quad (1)$$

$$n^{25\,°C}{}_D = 1.49362 + 0.003\,00x_1 + 0.000\,49x_1^2 \quad (2)$$

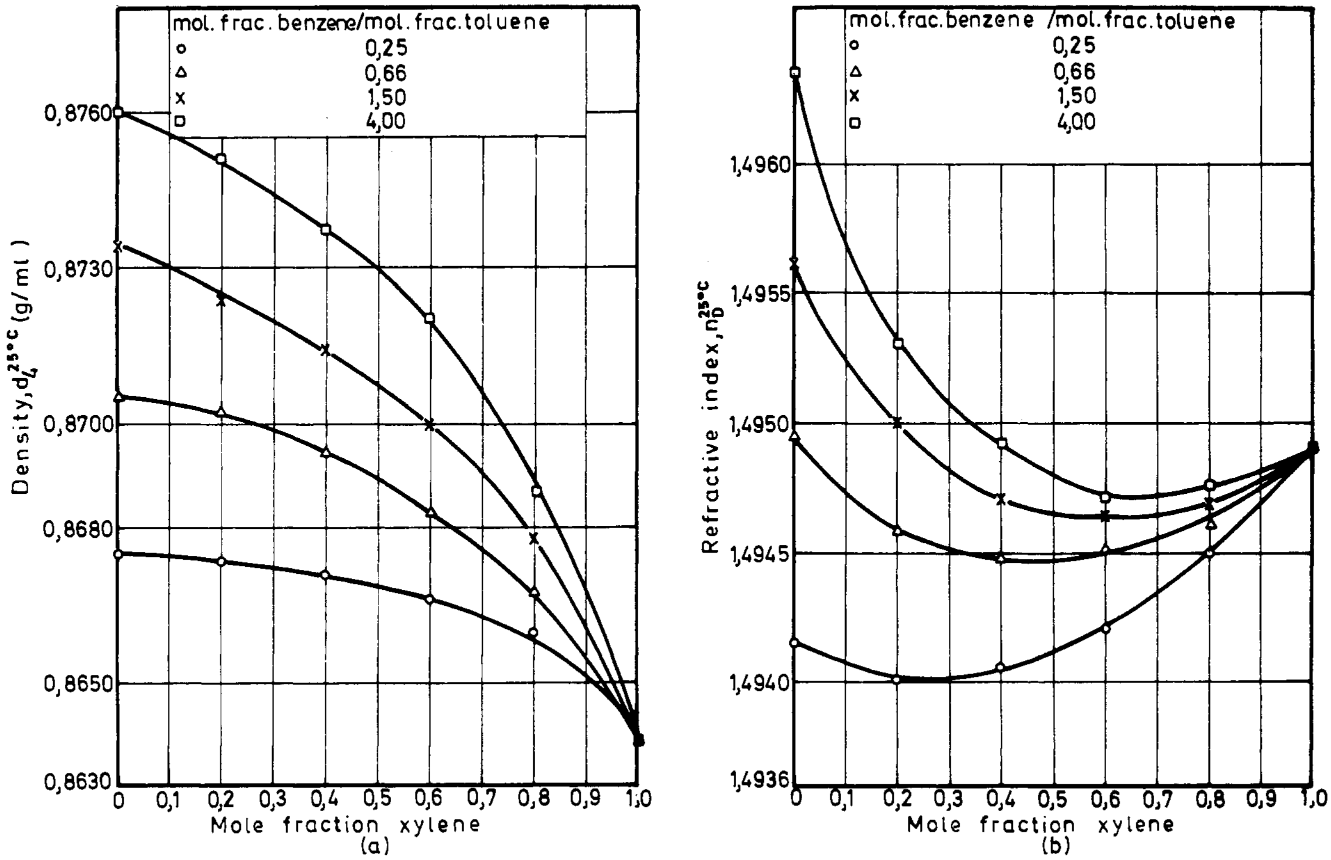

Figure 2. Densities (a) and refractive indices (b) of benzene–toluene–xylene system at 25 ± 0.005 °C.

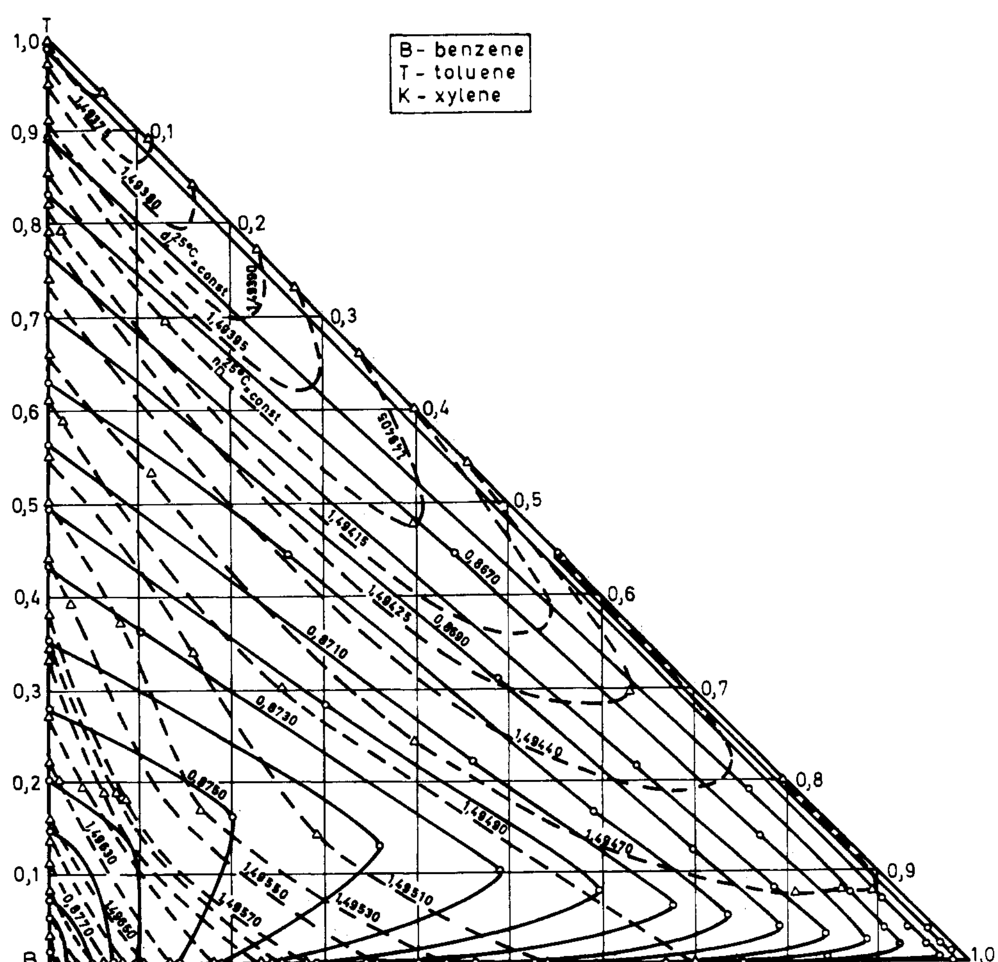

Figure 3. Densities and refractive indices of the benzene–toluene–xylene system with curves $d^{25\,°C}{}_4$ = constant and $n^{25\,°C}{}_D$ = constant.

Table V. Sum of Deviation Squares

Equation	Sum of deviation squares
1	0.1353×10^{-8}
2	$0.126\,08 \times 10^{-7}$
3	0.1783×10^{-5}
4	$0.141\,03 \times 10^{-8}$
5	0.4860×10^{-8}
6	$0.423\,14 \times 10^{-9}$
7	0.1539×10^{-4}
8	$0.370\,66 \times 10^{-5}$

Benzene–Xylene System:

$$d^{25\,°\mathrm{C}}{}_4 = 0.8640 + 0.0696x_1 - 0.9659x_1^2 + 4.7199x_1^3 - 9.9782x_1^4 + 9.5507x_1^5 - 3.3824x_1^6 \quad (3)$$

$$n^{25\,°\mathrm{C}}{}_\mathrm{D} = 1.494\,90 - 0.000\,43x_1 + 0.000\,76x_1^2 + 0.001\,87x_1^3 \quad (4)$$

Toluene–Xylene System:

$$d^{25\,°\mathrm{C}}{}_4 = 0.8639 + 0.0016x_2 - 0.0006x_2^2 \quad (5)$$

$$n^{25\,°\mathrm{C}}{}_\mathrm{D} = 1.494\,90 - 0.001\,34x_2 + 0.002\,38x_2^2 - 0.005\,16x_2^3 + 0.002\,87x_2^4 \quad (6)$$

Benzene–Toluene–Xylene System:

$$d^{25\,°\mathrm{C}}{}_4 = 0.8662 + 0.0132x_1 - 0.0012x_2 \quad (7)$$

$$n^{25\,°\mathrm{C}}{}_\mathrm{D} = 1.494\,62 + 0.002\,01x_1 - 0.001\,17x_2 \quad (8)$$

where x_1 = mole fraction of benzene and x_2 = mole fraction of toluene.

Table V presents the sum of deviation squares according to which the reliability of the calculated approximation could be proved. Equations 7 and 8 indicate that the highest deviations occur at both extreme concentrations (at the triangle apex), what usually would be expected.

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Refractive Index–Dry Substance Relationships for Commercial Corn Syrups

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A study of the relationship between refractive index and dry substance (total solids) has been made for a wide variety of commercial corn syrups (including high fructose corn syrup) and one maltodextrin. Dry substance levels from 0 to 85% and temperatures from 20 to 60 °C were covered in this study. The corn syrups and maltodextrin were produced by acid and dual conversion processes (the high fructose corn syrup process includes isomerization) and span a range of dextrose equivalent values from 12 to 95. Additional measurements to establish the dependence of the refractive index–dry substance relationship on ash content were made for ash levels from 0 to 1.5%. The results for 11 product types are presented in the form of tables and of mathematical equations for the purpose of converting refractive index measurements to dry substance contents. Ten commercial corn syrups and one maltodextrin were used.

A comprehensive study to establish accurate relationships between refractive index and dry substance content has been carried out for a wide variety of commercial corn syrups (including high fructose corn syrup) and one maltodextrin. This study included products made by acid conversion and dual conversion processes representative of products manufactured by the member companies of the Corn Refiners Association, Inc. (CRA). These products ranged in dextrose equivalent values from 12 to 95. Measurements were made for six or more dry substance levels from 15 to 85% and at temperatures of 20, 30, 45, and 60 °C for each of 11 products. Additional measurements were made on two commercial syrups which were ion exchange refined as well as on those syrups with added ash (up to 1.5% ash) to establish the dependence of the refractive index–dry substance relationships on ash content.

The resulting data for each product are available in tabular form from the Corn Refiners Association, Inc., 1001 Connecticut Avenue N.W., Washington, D.C., and have been filed with the ACS Microfilm Depository Service as supplementary tables (see paragraph at end of paper). These data have been fit by regression analysis to a suitable mathematical function for each of the 11 products. These functions have been used to generate detailed working tables which may be used for converting refractive index readings to dry substance values. Means of correcting for temperature and ash variations and for small variations in dextrose equivalent (D.E.) and/or product composition are included with these tables.

Analysis of the residuals (observed minus calculated values) indicates that the data are internally consistent and that a relatively simple mathematical model is capable of representing the relationships involved for a wide variety of product types. Careful work with sucrose and dextrose solutions and preliminary interlaboratory checks on several syrup samples served to establish the reliability and accuracy of the equipment and methods used by the investigators. Further mathematical analysis of the data reported here, aimed at establishing the relationship be-