attempt to prepare the Diels-Alder adduct of compound III with tetracyanoethylene failed. Apparently, an unstable π -complex did form however, since the reaction mixture assumed a persistent coloration, first red then brownish yellow, but only starting materials could be isolated. Recrystallization from ethanol gave the purified adduct (V) as fine, white needles, m.p. 227-229° (uncorr.). Anal. Calcd. for C₁₂H₁₂O₄: C, 65.45; H, 5.49; O, 29.06. Found: C, 65.47; H, 5.36; O, 28.87.

The infrared spectrum (see paragraph on infrared spectrum in section above) (potassium bromide wafer, 4 mg. per 200 mg.) exhibited C = C absorption at 6.08 (w), the cyclic ether band at 9.25 (s), as well as the components of the cyclic anhydride grouping characterized (2) by the broad, very strong absorptions of the carbonyl (doublet) at 5.40 to 5.65, and the C—O—C linkage centered at 8.20.

NMR data (10% in trifluoroacetic acid) showed these peaks: triplet at 3.47, 3.56, and 3.64 (2 vinyl protons); a multiplet between 5.74 and 6.43 (4 protons *ortho* to oxygen); a broad peak at 6.56 (4 protons at bridgehead and anhydride ring); and a multiplet at 7.18 (2 angular protons).

cis-2-OXAHEXAHYDROINDANE (cis-HEXAHYDROPHTHALAN)

A. From the Hydrogenation of Diolefin III. One gram of III in 1 ml. of ethanol was shaken with 100 mg. of 5% palladized charcoal catalyst for 3 hours at room temperature under 25 p.s.i.g. hydrogen pressure. Two equivalents of hydrogen were taken up. The catalyst was removed by filtration, washed with ethanol, and the combined filtrate and washings were fractionated. One gram of compound IV was obtained, b.p. 51° (8 mm. of Hg), $n_{\rm D}^{21}$ 1.4701, $n_{\rm D}^{25}$ 1.4683, d_4^{25} 0.9724 [lit. (4, 5) b.p. 59° (9 mm. of Hg), 179° (740 mm. of Hg), $n_{\rm D}^{21}$ 1.4712, $n_{\rm D}^{25}$ 1.4683, d_4^{25} 0.9727]. **B.** From the Hydrogenation of Monoolefin I. Ten grams of compound I, prepared by the method of Eliel and Pillar (3) b.p. $66.0-66.5^{\circ}$ (13.5 mm. of Hg), $n_{\rm D}^{25}$ 1.4890 [lit. (3) b.p. $63-64^{\circ}$ (13 mm. of Hg), $n_{\rm D}^{25}$ 1.4884], in 5 ml. of ethanol were hydrogenated in the same manner described for compound III; one equivalent of hydrogen was absorbed. Nine grams of IV were recovered, b.p. 51.5° (9 mm. of Hg), $n_{\rm D}^{25}$ 1.4680, $d_{\rm H}^{45}$ 0.9733.

The infrared spectra (neat, 0.0212 mm.) of the product derived from method A and method B were superimposable and corresponded with that of a published spectrum (4). Also, GLC analysis ($\frac{1}{4} \times 120$ inch column packed with 15% terephthalic acid-terminated Carbowax 20M supported on 60 to 80-mesh Chromosorb W) of a mixture of the two products gave a single peak.

ACKNOWLEDGMENT

The authors are indebted to Tom J. Mabry for his assistance in the interpretation of some of the NMR data and to Panayotis C. Petrellis for several helpful discussions. This work was supported by a research grant from the Robert A. Welch Foundation.

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RECEIVED for review November 1, 1963. Accepted October 26, 1964.

Refractive Indices of Some Ternary Systems Containing Naphthalene

Binary Solvent Mixtures Among Benzene, Toluene, Ethylbenzene, Carbon Tetrachloride

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Refractive indices have been determined at 25° C. for the ternary systems of naphthalene dissolved in the six solvent pairs from among benzene, toluene,ethylbenzene, and carbon tetrachloride; and for the various binary subsystems. Equations are given relating refractive index to solution composition in mole fraction. The average deviations in the ternary systems, from predicted refractive indices by these equations, range from 2 to 13×10^{-5} units among the systems. Only in the ethylbenzene-toluene-naphthalene and ethylbenzene-benzene-naphthalene ternary systems are deviations randomly distributed.

ANALYSIS, when performed using physical properties dependent upon the concentrations of all system components, grows more complex as the number of components increases. Graphical procedures, commonly used in relating a property to composition in a binary system, are generally not applicable in multicomponent systems. Analytical functions, although often impractical in hand calculations, may be conveniently used in analysis when

computer facilities are available. The present work illustrates the latter approach in representing the refractive indices, n, of some ternary systems containing naphthalene.

EXPERIMENTAL DATA

Equipment and procedure in determination of n, as well as the purity and n of the purified reagents, have been described in a previous study of naphthalene solubilities (3). The *n* value of liquid components differs from literature values by from 4 to 14×10^{-5} units. All *n* values in this study refer to $25.00 \pm 0.01^{\circ}$ C. and to the sodium D-line, 5893 A.

Binary system data are given in Table I. In liquid-solid binaries, the data extend to within 0.03 mole fraction of saturation. Ternary system data are given in Table II. More n were observed in a system (usually upward of 30) than the 20 that have been listed for each. Twenty points were considered adequate to furnish an indication of the behavior in each system. All data are from the region quite removed from the binaries. The points represent the extent of the concentration range covered, and they have been selected to include the values showing the greatest error in predicted n, as described below. Each system contains several points within a few hundredths mole fraction of naphthalene saturation.

REPRESENTATION OF DATA BY ANALYTICAL FUNCTIONS

Scatchard and Ticknor (6) have shown that in the ternary methanol-carbon tetrachloride-benzene system, n is expressible as a quadratic in component volume fractions. As one of the components in the present work is a solid, the volume fraction relation cannot be used because the

molal volume of supercooled naphthalene is not precisely known. Thus, mole fraction has been adopted despite a priori evidence (6) that this approach is less suitable.

It is proposed here that n of the binary systems be represented by

$$n = n_1 x_1 + n_2 x_2 + x_1 x_2 A_{12} \tag{1}$$

where n_i and x_i are the refractive index and mole fraction, respectively, of pure component *i*. A_{12} is a concentration dependent function defined by

$$A_{12} = B_{12} + C_{12} (x_1 - x_2) + D_{12} (x_1 - x_2)^2$$
(2)

where B_{12} , C_{12} , D_{12} are empirical constants evaluated from experimental *n* data. The constants of Equation 2 for the liquid-liquid binaries are listed in Table III.

Measured values of supercooled naphthalene n are not available. Estimation by atomic refractions is not possible because of the optical exaltation of naphthalene (2). Estimation by combining the accepted temperature coefficient of n (1) with n above the naphthalene melting point was rejected because of the work of Ward and Van Winkle (9). Their results indicate that this procedure may lead to considerable error.

For the ethylbenzene-naphthalene system, as interaction is small (3), n should vary linearly with volume fraction (6).

	Table I. R	efractive Indices	of Binary Systems at 25° C.		
System	Mole Fraction of First-named Component	Exptl. Refr. Index		Mole Fraction of First-named Component	Exptl. Refr. Index
Benzene-toluene	0.7567 0.6066 0.4457 0.2364 By Eq 1:Std. D Av. Dev. 10° =		Naphthalene-benzene	$\begin{array}{c} 0.2844 \\ 0.2638 \\ 0.2450 \\ 0.2377 \\ 0.2285 \\ 0.2243 \\ 0.2127 \end{array}$	$\begin{array}{c} 1.54312 \\ 1.54006 \\ 1.53736 \\ 1.53628 \\ 1.53502 \\ 1.53446 \\ 1.53279 \end{array}$
Benzene-ethylbenzene	0.8273 0.5877 0.4501 0.1835	$ \begin{array}{r} 1.49619\\ 1.49487\\ 1.49428\\ 1.49349\\ \begin{array}{r} 1.49349\\ \end{array} $		0.1561 0.0985 0.0489 By Eq. 1:Std. I Av. Dev. 10 ⁵ =	
	By Eq. 1:Std. Dev. $10^5 = 2$, Av. Dev. $10^5 = 2$		Naphthalene-toluene	$0.2884 \\ 0.2660$	$1.53601 \\ 1.53294$
Benzene–carbon tetrachloride	0.8297 0.6391 0.3684 0.2845 By Eq. 1:Std. I Av. Dev. 10 ⁵ =			0.2589 0.2511 0.2278 0.2129 0.1408 0.0978	$\begin{array}{c} 1.53197 \\ 1.53104 \\ 1.52767 \\ 1.52556 \\ 1.51518 \\ 1.50882 \end{array}$
Toluene-ethylbenzene	0.8230 0.6112 0.4165 0.1801 By Eq. 1:Std. 3		Naphthalene-ethylbenzene	0.0474 By Eq. 1:Std. J Av. Dev. 10 ⁵ = 0.2622 0.2449 0.2338	
Toluene-carbon tetrachlo r ide	Av. Dev. 10 ⁵ = 0.7735 0.5867 0.4297 0.2476 By Eq. 1:Std. 3	1.48718 1.48105 1.47536 1.46816		0.2163 0.1830 0.1237 0.0657 By Eq. 1:Std. 1 Av. Dev. 10 ⁵ =	$\begin{array}{c} 1.52198 \\ 1.51752 \\ 1.50962 \\ 1.50197 \\ \text{Dev. } 10^{\circ} = 3, \end{array}$
Ethylbenzene-carbon tetrachloride	Av. Dev. $10^5 =$ 0.8150 0.6358 0.4112 0.2201 By Eq. 1:Std. I Av. Dev. $10^5 =$	1 1.48825 1.48297 1.47533 1.46769 Dev. 10 ⁶ = 0,	Naphthalene-carbon tetrachloride	0.2395 0.2289 0.2231 0.2165 0.2010 0.1879 0.0791 By Eq. 1:Std. Av. Dev. 10 ⁵ =	

Table II. Refractive Indices of Ternary Systems at 25° C.

	Mole Mole Fraction of			Mole	Mole Fraction of	
System	Fraction of Second- First-named named Component Component	Exptl. Befr Index	System	Fraction of First-named Component	Second- named Component	Exptl. Refr. Index
Benzene-toluene-	0.1573 0.5888	1.53264	Toluene-ethylbenzene-	0.1220	0.6451	1.52479
naphthalene	0.2248 0.7261	1.50236	naphthalene	0.1159	0.6127	1.52991
	$\begin{array}{ccc} 0.2127 & 0.6871 \ 0.2017 & 0.6515 \end{array}$	$1.51016 \\ 1.51715$		$0.1693 \\ 0.1494$	$0.7708 \\ 0.6800$	$1.50152 \\ 1.51656$
	0.3098 0.4618	1.53038		0.1421	0.6469	1.52213
	$\begin{array}{ccc} 0.2908 & 0.4336 \\ 0.4219 & 0.5247 \end{array}$	$1.53746 \\ 1.50386$		$0.2995 \\ 0.3940$	$0.4281 \\ 0.5528$	$1.53114 \\ 1.50104$
	0.4041 0.5025	1.51014		0.3525	0.4945	1.51496
	0.3675 0.4570	1.52284		$0.3325 \\ 0.4702$	$0.4665 \\ 0.2962$	$1.52154 \\ 1.52675$
	$\begin{array}{rrrr} 0.5711 & 0.3704 \\ 0.5175 & 0.3356 \end{array}$	$1.50548 \\ 1.51947$		0.4489	0.2828	1.53149
	0.4923 0.3193	1.52586		0.5785	0.3681	1.50142
	$\begin{array}{ccc} 0.4714 & 0.2998 \\ 0.4438 & 0.2822 \end{array}$	$1.53186 \\ 1.53863$		$0.5174 \\ 0.4919$	$0.3292 \\ 0.3129$	$1.51569 \\ 1.52165$
	0.7067 0.2272	1.50761		0.7799	0.1677	1.50166
	$\begin{array}{rrr} 0.6829 & 0.2195 \\ 0.6531 & 0.2099 \end{array}$	$1.51270 \\ 1.51893$		$\begin{array}{c} 0.7418 \\ 0.7002 \end{array}$	$0.1595 \\ 0.1506$	$1.50836 \\ 1.51574$
	0.6218 0.1999	1.52542		0.6694	0.1440	1.52109
	$\begin{array}{rrrr} 0.7068 & 0.0596 \\ 0.6670 & 0.0562 \end{array}$	$1.53495 \\ 1.54113$		$0.6466 \\ 0.6036$	$0.1295 \\ 0.1209$	$1.52637 \\ 1.53343$
	Std. Dev. 10 ⁵ : 8(Eq. 3a), 15(1			Std. Dev. 10 ⁵ : 40		
	Av. Dev. 105: 7(Eq. 3a), 13(E			Av. Dev. 10 ⁵ : 2(
Benzene-ethylbenzene-	0.1177 0.6644	1.52345	Toluene-carbon tetra-	0.1672	0.6456	1.50293
naphthalene	$\begin{array}{ccc} 0.1106 & 0.6243 \\ 0.1734 & 0.7716 \end{array}$	$1.52980 \\ 1.50128$	chloride-naphthalene	$0.1633 \\ 0.1580$	$0.6303 \\ 0.6098$	$1.50652 \\ 1.51119$
	0.1645 0.7321	1.50803		0.2260	0.6870	1.48564
	$\begin{array}{ccc} 0.1542 & 0.6862 \\ 0.3180 & 0.4596 \end{array}$	$1.51578 \\ 1.52649$		$0.2085 \\ 0.3138$	$0.6336 \\ 0.4461$	$1.49911 \\ 1.51738$
	0.2978 0.4305	1.53335		0.4011	0.5325	1.48779
	0.4264 0.5209	1.50236		0.3722	0.4941	1.50002
	$\begin{array}{rrrr} 0.4031 & 0.4925 \\ 0.3817 & 0.4663 \end{array}$	$1.51000 \\ 1.51697$		$0.3482 \\ 0.5471$	$0.4622 \\ 0.3854$	$1.50997 \\ 1.49296$
	0.3583 0.4377	1.52440		0.5119	0.3606	1.50330
	$\begin{array}{rrrr} 0.4274 & 0.3004 \\ 0.5585 & 0.3918 \end{array}$	$1.53547 \\ 1.50279$		$0.4794 \\ 0.4803$	$0.3377 \\ 0.3339$	$1.51238 \\ 1.51257$
	0.5305 0.3722	1.51014		0.7262	0.2127	1.49729
	$\begin{array}{rrrr} 0.5037 & 0.3534 \\ 0.4788 & 0.3359 \end{array}$	$1.51694 \\ 1.52319$		$0.6845 \\ 0.6465$	$0.2004 \\ 0.1893$	$1.50600 \\ 1.51367$
	0.7823 0.1633	1.50548		0.6091	0.1784	1.52107
	$\begin{array}{rrrr} 0.7091 & 0.1480 \\ 0.6734 & 0.1406 \end{array}$	$1.51963 \\ 1.52621$		$0.6051 \\ 0.5858$	$0.1568 \\ 0.1518$	$1.52498 \\ 1.52857$
	0.6265 0.1194	1.53634		0.5780	0.1498	1.53001
	Std. Dev. 10 ⁵ :3(Eq. 3a), 5(E	q. 3b)		Std. Dev. 105: 19	9(Eq. 3a), 28	(Eq. 3b)
D	Av. Dev. 10 ⁵ :2(Eq. 3a), 4(Eq. 0.652)	-	Dahallan and and an	Av. Dev. 10 ⁵ : 13	-	-
Benzene-carbon tetra- chloride-naphthalene	$\begin{array}{cccc} 0.2598 & 0.6532 \\ 0.2394 & 0.6019 \end{array}$	$1.48704 \\ 1.50114$	Ethylbenzene-carbon tetrachloride-naph-	$0.1440 \\ 0.1354$	$0.6664 \\ 0.6266$	$1.50253 \\ 1.51133$
	0.2189 0.5504	1.51456	thalene	0.2016	0.7145	1.48408
	$\begin{array}{cccc} 0.2142 & 0.5296 \\ 0.3393 & 0.5816 \end{array}$	$1.51890 \\ 1.48864$		$\begin{array}{c} 0.1842 \\ 0.3379 \end{array}$	$0.6528 \\ 0.4872$	$1.49886 \\ 1.50538$
	0.3174 0.5442	1.50017		0.3173	0.4575	1.51371
	$\begin{array}{ccc} 0.3208 & 0.5091 \\ 0.2895 & 0.4595 \end{array}$	$1.50640 \\ 1.52094$		$0.3075 \\ 0.3797$	$0.4434 \\ 0.5436$	$1.51763 \\ 1.48889$
	0.5946 0.3357	1.49668		0.3545	0.5075	1.49940 1.51855
	$\begin{array}{ccc} 0.5601 & 0.3162 \\ 0.5210 & 0.2941 \end{array}$	$1.50662 \\ 1.51737$		$\begin{array}{c} 0.4871 \\ 0.4748 \end{array}$	$0.2826 \\ 0.2755$	$1.51855 \\ 1.52144$
	0.5185 0.2630	1.52367		0.5874	0.3365	1.49501
	$\begin{array}{ccc} 0.4841 & 0.2456 \\ 0.7879 & 0.1617 \end{array}$	$1.53192 \\ 1.50026$		$\begin{array}{c} 0.5530 \\ 0.5170 \end{array}$	0.3168	$1.50339 \\ 1.51198$
	0.7408 0.1520	1.51031		0.7559	$0.2962 \\ 0.1716$	1.49878
	0.7019 0.1440	1.51830		0.7064	0.1603	$1.50753 \\ 1.51422$
	$\begin{array}{ccc} 0.6658 & 0.1366 \\ 0.6330 & 0.1027 \end{array}$	$1.52547 \\ 1.53648$		$0.6680 \\ 0.6620$	$0.1516 \\ 0.1253$	1.51919
	0.7240 0.0456	1.53362		0.6314	0.1196	1.52427 1.52719
	0.6893 0.0434 Std. Dev. 10 ⁵ : 11(Eq. 3a), 24	1.53916 (Eq. 3b)		0.6138 Std. Dev. 10 ⁵ : 1	0.1162 0(Eq. 3a) - 30	1.52719 (Eq. 3b)
	Av. Dev. 10^5 : 9(Eq. 3a), 19(I			Av. Dev. 10 ⁵ : 8(
	· · · · ·	-				• *

Moreover the molar volume of dissolved naphthalene is 123 ml. at 20° C. (4), and that of ethylbenzene is 123.06 ml. at 25° C. (5). Linearity of n with mole fraction should therefore also be obtained. A plot of n vs. mole fraction is precisely linear from 0 to 0.2662 mole fraction naphthalene in this system, the latter concentration being near saturation. Accordingly, the value of supercooled naphthalene n at 25° C. assigned here is that obtained by extrapolation of this plot to pure supercooled naphthalene, 1.62615. On this

basis, B_{12} , C_{12} , D_{12} values for the naphthalene-solvent systems are also included in Table III. The standard and average deviations of the experimental n from those predicted with Equation 1 are listed in Table I.

As the first approximation to ternary behavior, the equation

$$n = n_1 x_1 + n_2 x_2 + n_3 x_3 + x_1 x_2 A_{12} + x_1 x_3 A_{13} + x_2 x_3 A_{23}$$
(3)

is proposed. Differences between experimental n and those

Table III. Binary System Constants

	Constants of Equation 2 (x ₁ is First-named Component)				
System	B_{12}	C_{12}	D_{12}		
Benzene-toluene	-0.00260	-0.00029	-0.00112		
Benzene-ethylbenzene	-0.00397	-0.00131	-0.00137		
Benzene-carbon					
tetrachloride	0.00029	0.00013	-0.00124		
Toluene-ethylbenzene	-0.00056	-0.00032	-0.00123		
Toluene-carbon					
tetrachloride	0.00877	-0.00125	-0.00165		
Ethylbenzene-carbon					
tetrachloride	0.01291	-0.00256	-0.00039		
Naphthalene-benzene	0.03063	-0.03571	-0.01649		
Naphthalene-toluene	0.00669	-0.04113	-0.03218		
Naphthalene-ethylbenzene	0	0	0		
Naphthalene-carbon					
tetrachloride	-0.03188	-0.29878	-0.25816		

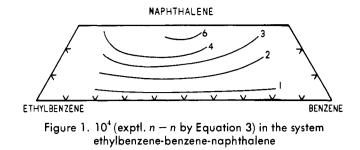
calculated with Equation 3 are considerable. The system showing the smallest differences is given in Figure 1. The differences range to a maximum of 50×10^{-4} units in the systems containing carbon tetrachloride. In the latter, the differences show considerable liquid-liquid asymmetry. To fit the differences, Equation 3 has been expanded to an Equation 3a, which includes a ternary deviation function, $x_1x_2x_3A_{123}$, where

$$A_{123} = B_{123} + C_{123}x_1 + D_{123}x_2 + E_{123}x_1^2 + F_{123}x_2^2 + G_{123}x_1x_2$$
(4)

In addition, an Equation 3b has been considered, in which the fifth order term coefficients of Equation 4 (E_{123} , F_{123} , G_{123}) are assigned a zero value. Table II lists the standard and average deviations of the experimental *n* from those predicted with Equations 3a and 3b. Constants used in these equations are given in Table IV.

As there is greater interaction between carbon tetrachloride and naphthalene than between the latter and the other solvents (3), Equation 3 was modified for the systems containing carbon tetrachloride by an approach described by Scatchard and coworkers (7). This amounts to replacement in the ternary system of the quantity $(x_i - x_j)$ by $(2x_i - 1)$ where x_i refers to the component whose property is in considerable contrast to those of the other two components. Results by this approach were in greater error than those obtained using Equation 3 itself.

Computations in the present work were programmed for a digital computer. The most complex aspect, evaluation of constants in the n vs. composition equations, involved obtaining solution matrices through inversion of those matrices formed in least-squares treatment of the experimental n and composition data pairs.



DISCUSSION

Differences between experimental and calculated n are uniformly small in the binary liquid-liquid systems, approximating the inherent instrument limitation, about $\pm 3 \times 10^{-5}$ units. In the binary systems containing naphthalene, the differences are somewhat greater. The greatest difference in any single experimental binary n is 19×10^{-5} units.

An apparent difference in behavior between the liquidliquid and solid-liquid binaries—indicated by the contrast in Table III of C_{12}/B_{12} that are small for the former and large for the latter—should be disregarded. This is the result of fitting the data over a restricted concentration range in the latter systems.

In the ternary systems, n calculated with Equation 3 are systematically below the experimental values in all present systems. The extent of the disagreement reflects the difference in n_i of the pure liquids.

In the present systems, Equations 3a and 3b appear to lead to significant results in representing the data. Errors in applying these equations in a given system show a comparable systematic trend, however, except in the benzene- and toluene-ethylbenzene mixed solvent systems, where the errors appear to be random. Both the average and extreme differences in the other systems are greater by Equation 3b than by 3a. With the former and latter, respectively, the greatest differences in any single ternary system are 60 and 40×10^{-5} units.

No consideration to equations other than those proposed above has been given in the present work. Others may be more suitable. Thus it appears probable that an empirical expression for n in terms of a power series in x_i and x_j might be obtainable. In fact, Equation 1 for binary systems reduces to such a form, with no cross terms in x_1x_2 . Power series have been used for this purpose in binary systems. A quadratic expression in solute concentration is sufficient over a considerable concentration range even for some systems of electrolytes in water (8). However, combination of the pertinent quadratics for the binaries into a suitable form

		100.011.	Ternary Sy						
	Equation 3a					Equation 3b			
System	B_{123}	C_{123}	D_{123}	$E_{_{123}}$	${m F}_{123}$	$G_{\scriptscriptstyle 123}$	B_{123}	$C_{_{123}}$	D_{123}
Benzene-toluene-naphthalene	0.8075	-1.7337	-1.6898	0.9412	0.8877	1.9111	0.1586	-0.1528	-0.1481
Benzene-ethylbenzene-naphthalene	0.2778	-0.6442	-0.5718	0.3956	0.3209	0.6672	0.0374	-0.0323	-0.0208
Benzene-carbon tetrachloride-									
naphthalene	2.0742	-3.7785	-4.4542	1.8343	2.3967	4.1429	0.7044	-0.5899	-0.8406
Toluene-ethylbenzene-naphthalene	0.2067	-0.4174	-0.3710	0.2138	0.1940	0.3879	0.0672	-0.0735	-0.0435
Toluene-carbon tetrachloride-									
naphthalene	1.8879	-3.3782	-4.1546	1.5647	2.2498	3.8422	0.5987	-0.5015	-0.7303
Ethylbenzene-carbon tetra- chloride-naphthalene	2.2320	-4.2015	-5.0901	2.0583	2.8616	4.8559	0.5799	-0.4939	-0.7346

subscripts 1,2,3 refer to the components in the order listed in

Column 1 of this table.

for the resultant ternaries was not possible. The comparative magnitudes of B_{123} , C_{123} , etc. in Table IV, where only the deviations from Equation 3 were to be fitted, indicate that a rather large number of terms might be needed in an effective power series for these ternary systems.

The present approach to an analytical function for the ternary data would be quite unwieldy without the use of a computer. For example, the determination of an unknown composition by locating the intersection of two functions of the form of Equation 3a or 3b for two different physical properties would require extensive iterative procedures.

ACKNOWLEDGMENT

This work was supported in part by the Petroleum Research Fund administered by the American Chemical Society. Linda Gladin and the University of Georgia Institute of Statistics provided vital assistance in computation.

NOMENCLATURE

- A_{ii} = function defined in Equation 2
- A_{iik} = function defined in Equation 4

 $B_{i_i}, C_{i_i}, D_{i_i}$ = constants in Equation 2

- $B_{ijk}, C_{ijk}, D_{iik}, E_{ijk}, F_{ijk}, G_{ijk} = \text{constants in Equation 4}$ n = refractive index
 - n_i = refractive index of pure component *i*
 - x_i = mole fractive index of pure component *i*

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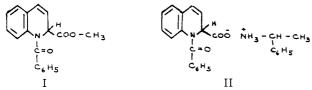
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RECEIVED for review May 6, 1964. Accepted November 2, 1964.

Derivatives of 1-Benzoyl-1,2-dihydroquinaldic Acid (Reissert Acid)

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KEISSERT ACID (1-benzoyl-1,2-dihydroquinaldic acid) was prepared by the method of Collins and Henshall (1), during an investigation of the chemistry of Reissert compounds. Two derivatives of this acid were prepared namely, methyl 1-benzoyl-1,2-dihydroquinaldate (I) and d- α -methylbenzylammonium 1-benzoyl-1,2-dihydroquinaldate (II).



The methyl ester, I, was obtained as a crystalline solid by treating a methanol solution of 1-benzoyl-1,2-dihydroquinaldic acid with an excess of diazomethane in ether. The crystalline ammonium salt, II, was obtained by the reaction of 1-benzoyl-1,2-dihydroquinaldic acid with d- α phenylethylamine in anhydrous acetone.

EXPERIMENTAL

Elemental analyses were carried out by Schwarzkopf Microanalytical Laboratory, Woodside, N.Y. All melting points are corrected.

Methyl 1-Benzoyl-1,2-dihydroquinaldate. To a solution of 3.0 grams (0.01 mole) of 1-benzoyl-1,2-dihydroquinaldic acid in 25 ml. of absolute methanol cooled in an ice bath,

an excess, as noted by the yellow color of the solution, of an ice cold ether solution of freshly prepared diazomethane was added slowly (2). When the evolution of nitrogen had ceased, the solution was warmed to room temperature and the solvents distilled, the latter portion under reduced pressure. This gave 2.1 grams (67.1%) of a light yellow solid, m.p. 115–118°C. Recrystallization from methanol gave a white crystalline solid, m.p. 118–119°C.

Anal. Calcd. for $C_{18}H_{15}NO_3$: C, 73.72; H, 5.15; N, 4.77. Found: C, 73.82; H, 5.33; N, 5.00.

d- α -Methylbenzylammonium aldate. A solution of 0.5 gram (0.0017 mole) of 1-benzoyl-1,2-dihydroquinaldic acid in 5 ml. of absolute acetone was mixed with 0.21 gram (0.0017 mole) of d- α -phenylethylamine (3). The solution was warmed on a steam bath for one to two minutes and cooled. In approximately one-half hour, a white solid precipitated from solution. This was filtered and washed with acetone, m.p. 168–169.6° C.

Anal. Calcd. for $C_{25}H_{24}N_2O_3;\ C,\ 75.03;\ H,\ 6.04;\ N,\ 7.00.$ Found: C, 75.15; H, 6.06; N, 7.24.

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RECEIVED for review July 6, 1964. Accepted November 16, 1964.