J. M. Sørensen
W. Arlt

LIQUID-LIQUID EQUILIBRIUM DATA COLLECTION

Ternary Systems

Chemistry Data Series
Vol. V, Part 2

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PREFACE OF AUTHORS

This work consists of three Parts. Part 1 deals with binary liquid-liquid equilibria and Parts 2 and 3 with ternary liquid-liquid equilibria.

The correlation and prediction of liquid-liquid equilibria (LLE) using models for liquid phase non-idealities is a subject within chemical engineering which is not yet mastered quantitatively. Model inadequacies may be one explanation for this. However, this work will show that the results may be quite good with existing models if they are used properly, i. e. if the parameter estimation procedure as well as the data base are chosen carefully.

In addition to an extensive collection of experimental binary, ternary, and quaternary data, this work contains NRTL and UNIQUAC parameters reduced from these data. For each ternary system (Parts 2 and 3) we give a specific set of NRTL and UNIQUAC parameters which emphasizes the distribution ratio of the solute at small concentrations. This makes semi-quantitative extraction calculations possible for many systems. We also include a table of UNIQUAC parameters for the A-B interaction reduced from a large number of systems with components A, B, and any third component. These parameters will usually be better for predicting multicomponent LLE than parameters based on VLE-data.

The work leading to these three books began in 1977 at Instituttet for Kemiteknik, Lyngby, Denmark, where Aa. Fredenslund started a project called "A Group Contribution Method for Predicting Liquid-Liquid Equilibria". An initial step in this project was to investigate how existing molecular models (e.g. NRTL and UNIQUAC) behave in LLE calculations. For this purpose a parameter estimation procedure and a large data base were established.

The above project was close to research plans at Dortmund University, and a collaboration was initiated in 1978 with the purpose of jointly preparing this publication. The data collection was extended, and the authors have profited very much by the experience of J. Gmehling and U. Onken who started Volume I of this series („Vapor-Liquid Equilibrium Data Collection").

Simultaneously the parameter estimation procedure was further refined under daily guidance of Aa. Fredenslund and P. Rasmussen to whom the authors are very grateful.

The parameter estimation from ternary LLE-data involves many numerical problems. The authors wish to thank M. L. Michelsen (Instituttet for Kemiteknik, Lyngby) for providing the final version of the estimation procedure. Finally, we dedicate special thanks to T. Magnussen (DECHEMA, Frankfurt/Main) for many fruitful discussions and help and to colleagues and students in Lyngby and Dortmund for various kinds of assistance.

The authors hope that the data collection and parameters of this work will be of use to the industry. We also hope that the availability of the large amount of data will facilitate the testing of new models at universities.

The authors

PREFACE OF EDITORS

Subjects of the DECHEMA Chemistry Data Series are the physical and thermodynamic property data of chemical compounds and mixtures essentially for the fluid state covering PVT data, heat capacity, and entropy data, phase equilibrium data, transport and interfacial tension data.

The main purpose is to provide chemists and engineers with data for process design and development. For computer based calculations in process design appropriate correlation methods and accurate data must be used. These are only in some cases available in open literature. For that reason the most urgent requirement regarding the publication of data is to offer critically evaluated and reliable data. This will be the goal of the series.

DECHEMA gives an opportunity to authors especially from universities to publish not only their theoretical results, but also their measured or compiled data, most often a large amount.

After that a successful group contribution method for the prediction of vapor-liquid equilibria (UNIFAC) had been presented to the scientific community several years ago, the needs for a similar treatment of liquid-liquid equilibria led to a cooperation between the Dechema Data Compiler Development Group and Professor Fredenslund at the Instituttet for Kemiteknik in Lyngby, who has much experience in this field.

During this cooperation, J. M. Sørensen and W. Arlt, who is already co-author of Volume I of the Series, have collected the mutual solubility data of more than 2000 binary, ternary and quaternary mixtures of organic liquids.

This compilation is now being published as Volume V of this series, in 3 parts giving not only measured data but also evaluated correlation constants and recommended values. We hope that this gives an instrument that will allow the users to solve their problems considerably more easily aid more quickly than before.

Frankfurt/Main, October 1980

Dieter Behrens
Reiner Eckermann

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Vol. V, Part 2

(1) C6H15N AMINE,TRIETHYL

(2) CCL4 METHANE,TETRACHLORO

(3) C2H4O2 ACETIC ACID

PLEKHOTKIN V.F., MARKUZIN N.P.
FIZ.KHIM.SVOISTVA RASTVOROV,LENINGRAD,EDITOR:A.I.RUSANOV
(1964)12

TEMPERATURE = 20.0 DEG C TYPE OF SYSTEM = 1

EXPERIMENTAL TIE LINES IN MOLE PCT

LEFT PHASE			RIGHT PHASE		
(1)	(2)	(3)	(1)	(2)	(3)
93.400	0.0	6.600	41.000	0.0	59.000
91.400	2.000	6.600	41.200	0.900	57.900
88.700	4.600	6.700	41.300	2.000	56.700
86.100	7.100	6.800	41.400	3.400	55.200
82.000	11.100	6.900	41.500	5.300	53.200
77.000	14.400	8.600	41.800	7.100	51.100
72.700	17.200	10.100	42.300	8.900	48.800
69.800	19.200	11.000	42.300	10.400	47.300
65.800	20.900	13.300	42.500	11.700	45.800
64.200	21.600	14.200	42.500	13.500	44.000
62.000	22.200	15.800	42.500	14.700	42.800
58.000	22.900	19.100	43.400	16.700	39.900

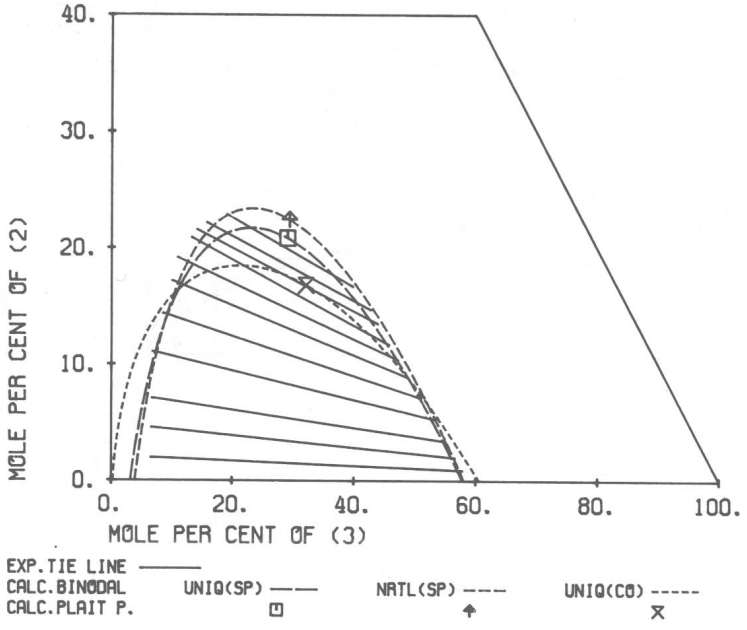
SPECIFIC MODEL PARAMETERS IN KELVIN

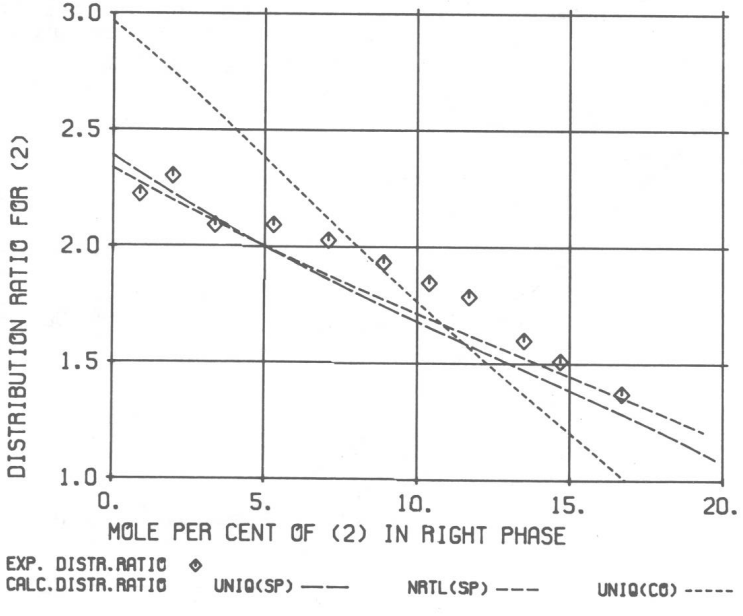
		UNIQUAC		NRTL(ALPHA=.2)	
I	J	AIJ	AJI	AIJ	AJI
1	2	269.73	-226.60	-303.24	90.369
1	3	766.22	-159.96	1162.9	-143.69
2	3	251.77	-34.635	350.19	75.515

R1 = 5.0118 R2 = 3.3900 R3 = 2.2024
Q1 = 4.256 Q2 = 2.910 Q3 = 2.072

MEAN DEV. BETWEEN CALC. AND EXP. CONC. IN MOLE PCT

UNIQUAC (SPECIFIC PARAMETERS)	1.03
NRTL (SPECIFIC PARAMETERS)	0.69
UNIQUAC (COMMON PARAMETERS)	2.02





CCl_4-$C_2H_4O_2$

(1) H2O WATER

(2) C2H4O2 ACETIC ACID

(3) CCL4 METHANE,TETRACHLORO

KRISHNAMURTY V.V.G., MURTI P.S., VENKATA RAO C.
J.SCI.IND.RES. 12B(1953)583

TEMPERATURE = 27.5 DEG C TYPE OF SYSTEM = 1

EXPERIMENTAL TIE LINES IN MOLE PCT

LEFT PHASE			RIGHT PHASE		
(1)	(2)	(3)	(1)	(2)	(3)
87.168	12.802	0.030	0.0	4.485	95.515
77.140	22.679	0.181	0.0	8.501	91.499
69.513	29.978	0.509	0.0	11.880	88.120
55.587	42.460	1.953	0.759	17.082	82.159
52.296	45.181	2.523	1.472	20.531	77.997

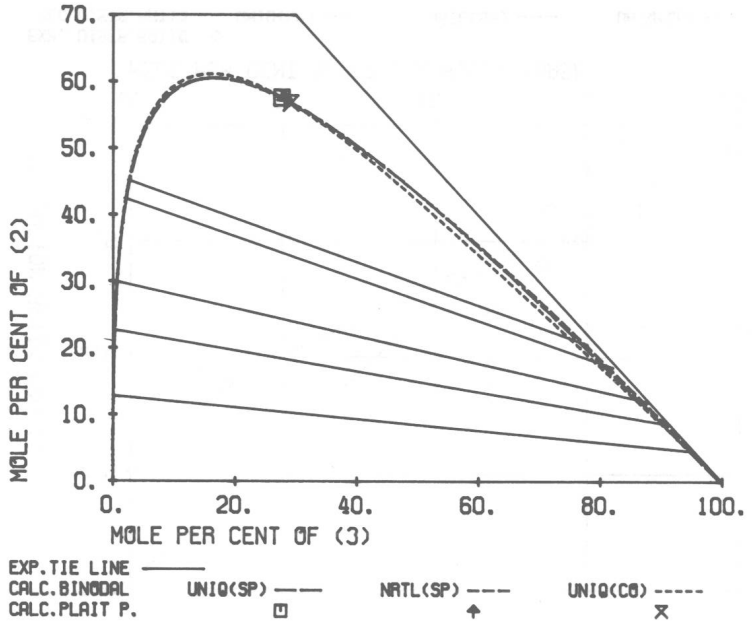
SPECIFIC MODEL PARAMETERS IN KELVIN

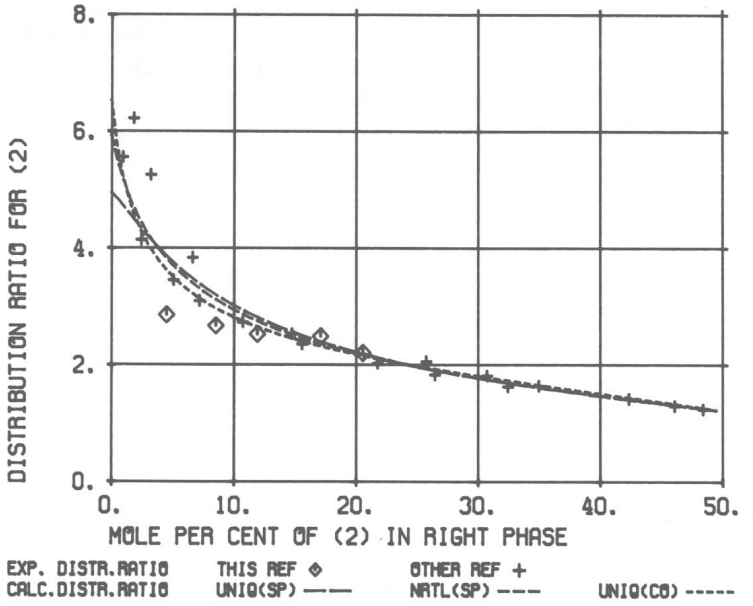
		UNIQUAC		NRTL(ALPHA=.2)	
I	J	AIJ	AJI	AIJ	AJI
1	2	-238.97	-48.556	185.08	-374.61
1	3	525.57	861.16	2102.8	1267.2
2	3	29.822	60.388	473.17	-92.441

R1 = 0.9200 R2 = 2.2024 R3 = 3.3900
Q1 = 1.400 Q2 = 2.072 Q3 = 2.910

MEAN DEV. BETWEEN CALC. AND EXP. CONC. IN MOLE PCT

UNIQUAC (SPECIFIC PARAMETERS)	0.87
NRTL (SPECIFIC PARAMETERS)	0.78
UNIQUAC (COMMON PARAMETERS)	1.12





2
CCl_4-$C_2H_4O_2$

(1) H2O	WATER
(2) C2H4O2	ACETIC ACID
(3) CCL4	METHANE,TETRACHLORO

PRINCE R.G.H., HUNTER T.G.
CHEM.ENG.SCI. 6(1957)245

TEMPERATURE = 25.0 DEG C TYPE OF SYSTEM = 1

EXPERIMENTAL TIE LINES IN MOLE PCT

LEFT PHASE			RIGHT PHASE		
(1)	(2)	(3)	(1)	(2)	(3)
94.873	5.088	0.039	0.170	0.916	98.915
89.896	10.030	0.074	0.168	2.419	97.413
82.393	17.429	0.178	0.248	5.053	94.699
77.442	22.233	0.325	0.326	7.180	92.495
70.156	29.187	0.657	0.556	10.695	88.749
62.143	36.578	1.279	0.767	15.557	83.676
53.412	44.123	2.465	1.315	21.747	76.938
47.939	48.469	3.592	1.757	26.445	71.798
41.883	52.743	5.374	2.790	32.399	64.812

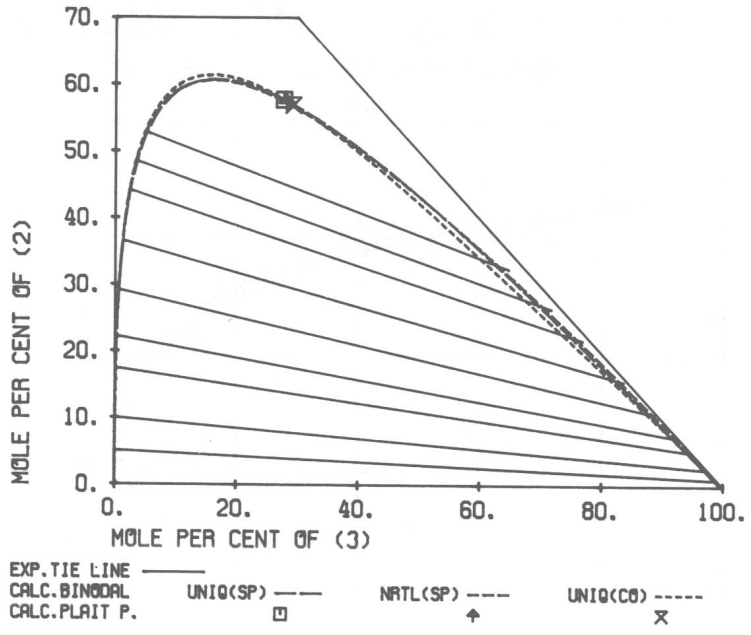
SPECIFIC MODEL PARAMETERS IN KELVIN

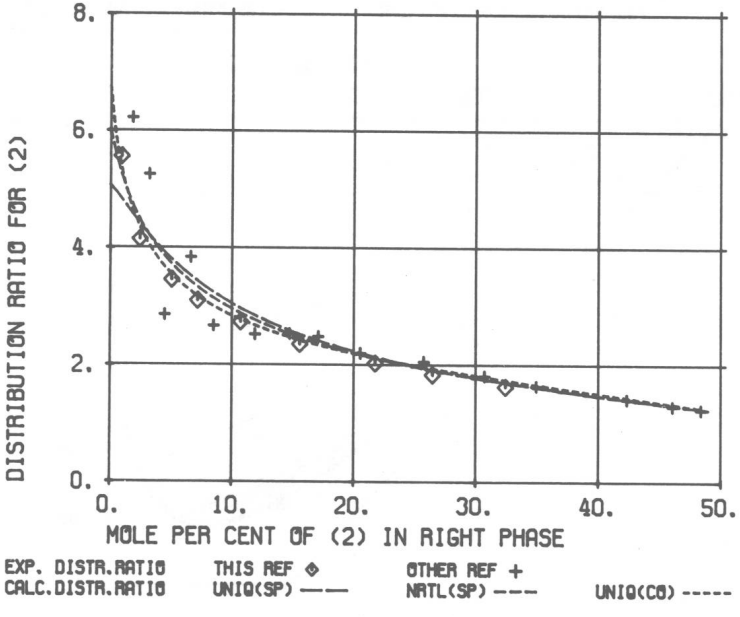
	UNIQUAC		NRTL(ALPHA=.2)	
I J	AIJ	AJI	AIJ	AJI
1 2	-238.97	-48.556	185.08	-374.61
1 3	525.57	861.16	2102.8	1267.2
2 3	29.822	60.388	473.17	-92.441

R1 = 0.9200 R2 = 2.2024 R3 = 3.3900
Q1 = 1.400 Q2 = 2.072 Q3 = 2.910

MEAN DEV. BETWEEN CALC. AND EXP. CONC. IN MOLE PCT

UNIQUAC (SPECIFIC PARAMETERS)	0.73
NRTL (SPECIFIC PARAMETERS)	0.59
UNIQUAC (COMMON PARAMETERS)	0.86





CCl_4-$C_2H_4O_2$

(1) H2O WATER

(2) C2H4O2 ACETIC ACID

(3) CCL4 METHANE,TETRACHLORO

FUSE K., IGUCHI A.
KAGAKU KOGAKU 34(1970)1001

TEMPERATURE = 25.0 DEG C TYPE OF SYSTEM = 1

EXPERIMENTAL TIE LINES IN MOLE PCT (GRAPH.INTERPOL.)

LEFT PHASE			RIGHT PHASE		
(1)	(2)	(3)	(1)	(2)	(3)
88.724	11.157	0.119	0.421	1.792	97.787
83.004	16.798	0.198	0.666	3.196	96.139
74.203	25.378	0.418	1.135	6.617	92.248
61.713	37.261	1.026	2.280	14.729	82.991
42.377	53.023	4.600	3.735	25.733	70.532
38.137	55.713	6.150	4.489	30.700	64.811
34.651	57.439	7.910	5.190	34.935	59.875
27.621	60.101	12.277	6.331	42.326	51.292
26.395	59.955	13.650	7.372	46.073	46.555
23.852	50.064	16.084	8.307	48.383	43.310

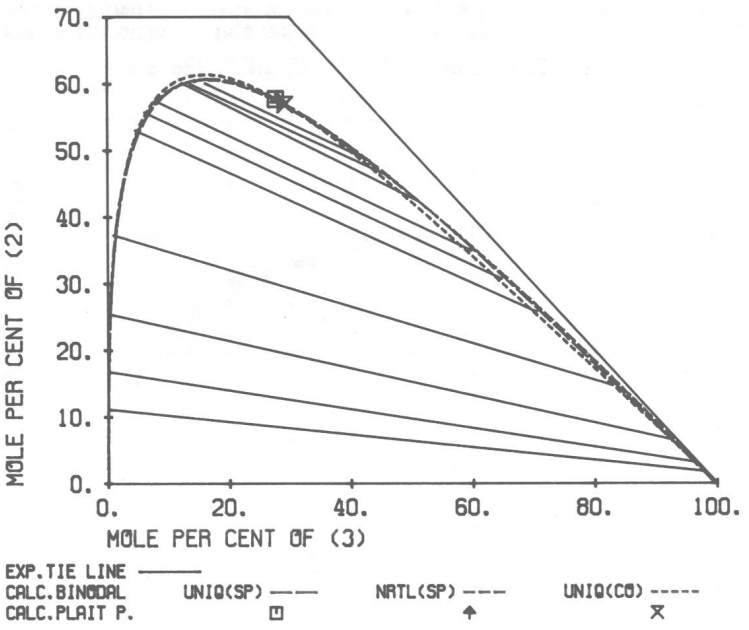
SPECIFIC MODEL PARAMETERS IN KELVIN

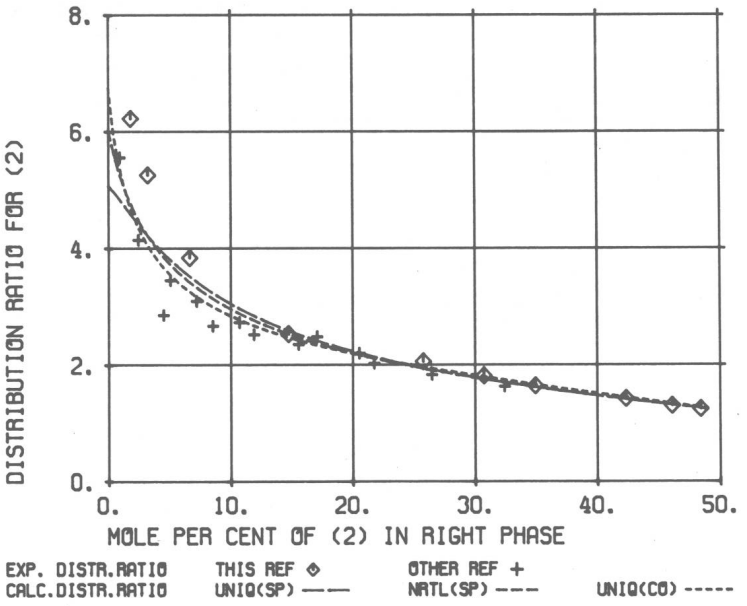
		UNIQUAC		NRTL(ALPHA=.2)	
I	J	AIJ	AJI	AIJ	AJI
1	2	-238.97	-48.556	185.08	-374.61
1	3	525.57	861.16	2102.8	1267.2
2	3	29.822	60.388	473.17	-92.441

R1 = 0.9200 R2 = 2.2024 R3 = 3.3900
Q1 = 1.400 Q2 = 2.072 Q3 = 2.910

MEAN DEV. BETWEEN CALC. AND EXP. CONC. IN MOLE PCT

UNIQUAC (SPECIFIC PARAMETERS)	0.64
NRTL (SPECIFIC PARAMETERS)	0.66
UNIQUAC (COMMON PARAMETERS)	0.90





(1) C3H8O3 GLYCEROL

(2) C2H6O ETHANOL

(3) CCL4 METHANE,TETRACHLORO

MCDONALD H.J., KLUENDER A.F., LANE R.W.
J.PHYS.CHEM. 46(1942)946

TEMPERATURE = 25.0 DEG C TYPE OF SYSTEM = 1

EXPERIMENTAL TIE LINES IN MOLE PCT

LEFT PHASE			RIGHT PHASE		
(1)	(2)	(3)	(1)	(2)	(3)
90.782	8.643	0.575	0.166	0.994	98.840
76.472	21.687	1.840	0.312	9.348	90.340
63.028	33.053	3.919	1.036	15.679	83.285
51.176	41.964	6.860	2.052	24.620	73.328
43.293	46.377	10.330	8.428	39.239	52.333

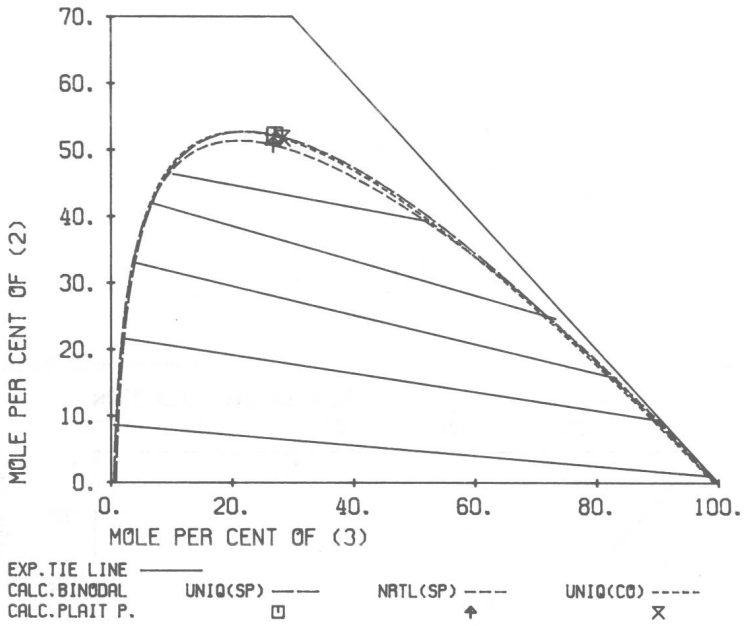
SPECIFIC MODEL PARAMETERS IN KELVIN

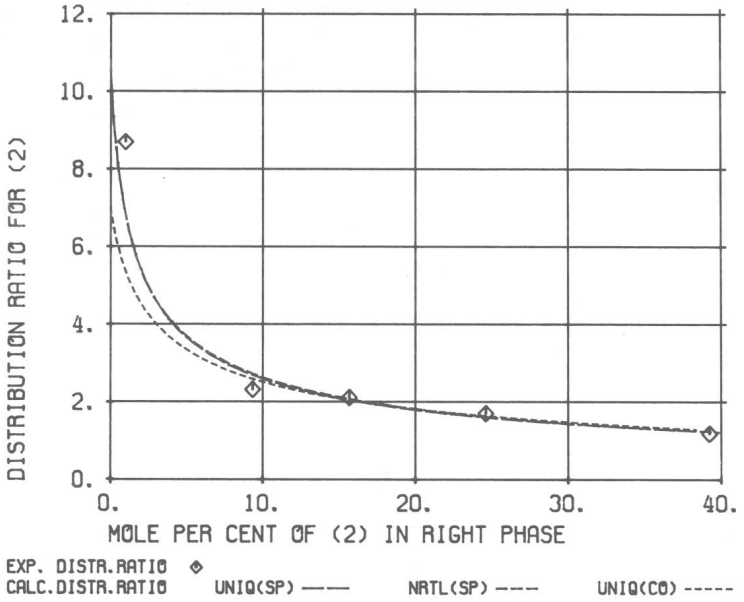
		UNIQUAC		NRTL(ALPHA=.2)	
I	J	AIJ	AJI	AIJ	AJI
1	2	-9.5920	-274.21	-181.37	-468.95
1	3	300.09	329.12	1039.6	1426.6
2	3	74.791	-165.69	545.76	-497.24

R1 = 3.5857 R2 = 2.1055 R3 = 3.3900
Q1 = 3.060 Q2 = 1.972 Q3 = 2.910

MEAN DEV. BETWEEN CALC. AND EXP. CONC. IN MOLE PCT

UNIQUAC (SPECIFIC PARAMETERS)	1.22
NRTL (SPECIFIC PARAMETERS)	1.09
UNIQUAC (COMMON PARAMETERS)	1.38





CCl_4-C_2H_6O

(1) H2O WATER

(2) C2H6O ETHANOL

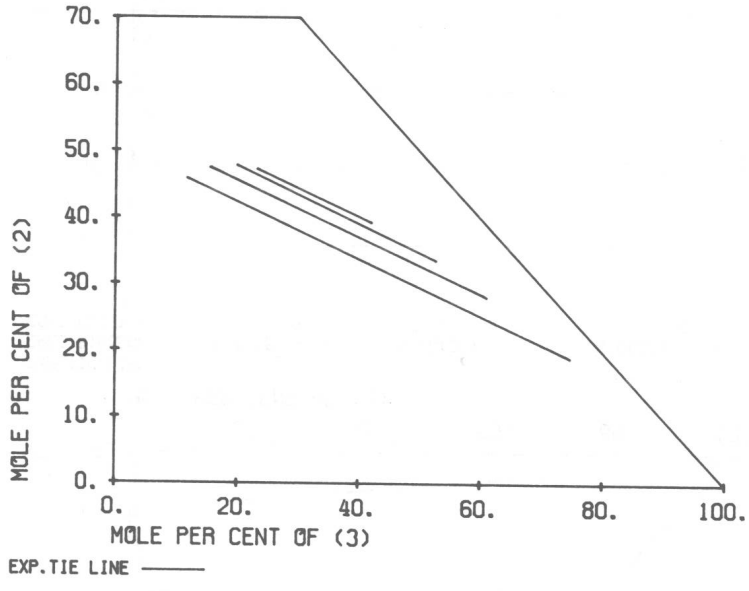
(3) CCL4 METHANE,TETRACHLORO

BONNER W.D.
J.PHYS.CHEM. 14(1910)738

TEMPERATURE = 0.0 DEG C TYPE OF SYSTEM = 1

EXPERIMENTAL TIE LINES IN MOLE PCT (GRAPH.INTERPOL.)

LEFT PHASE			RIGHT PHASE		
(1)	(2)	(3)	(1)	(2)	(3)
42.518	45.823	11.659	6.240	18.977	74.783
37.142	47.429	15.429	10.869	28.099	61.032
32.397	47.759	19.844	13.742	33.532	52.726
29.595	47.244	23.162	18.654	39.277	42.069



(1) CCL4 METHANE,TETRACHLORO

(2) C3H6O 2-PROPANONE

(3) H2O WATER

BUCHANAN R.H.
IND.ENG.CHEM. 44(1952)2449

TEMPERATURE = 30.0 DEG C TYPE OF SYSTEM = 1

EXPERIMENTAL TIE LINES IN MOLE PCT (GRAPH.INTERPOL.)

LEFT PHASE			RIGHT PHASE		
(1)	(2)	(3)	(1)	(2)	(3)
97.826	2.090	0.084	0.028	1.066	98.906
89.959	9.801	0.240	0.032	3.447	96.521
88.391	11.292	0.317	0.034	3.884	96.081
67.812	29.146	3.042	0.056	8.209	91.736
62.979	33.194	3.827	0.059	9.141	90.800
50.966	43.629	5.405	0.090	12.012	87.899
39.686	53.525	6.789	0.189	14.956	84.854
32.153	57.861	9.987	0.286	17.626	82.087
23.479	60.132	16.388	0.468	21.776	77.756
18.418	59.892	21.690	0.844	25.028	74.128

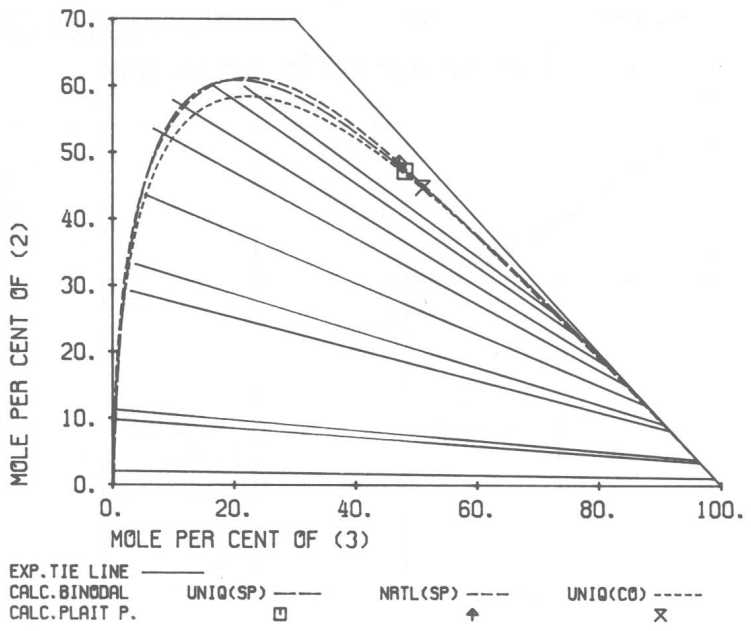
SPECIFIC MODEL PARAMETERS IN KELVIN

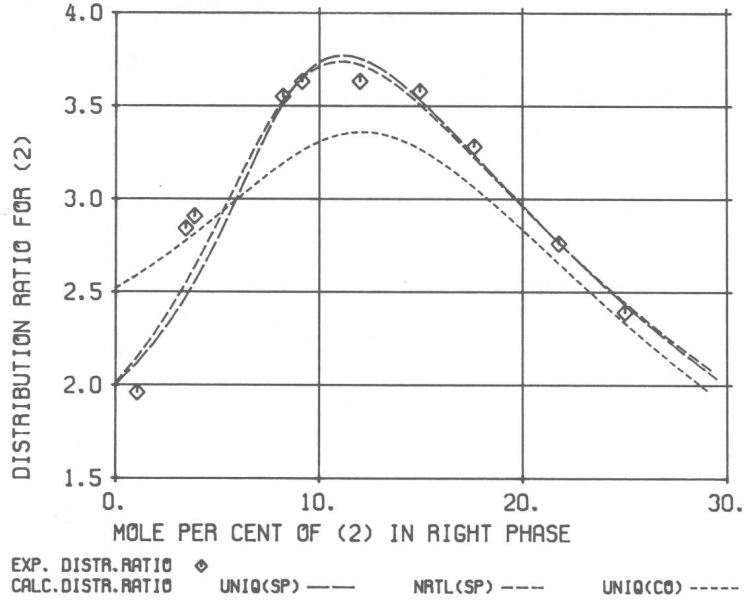
		UNIQUAC		NRTL(ALPHA=.2)	
I	J	AIJ	AJI	AIJ	AJI
1	2	358.93	-141.50	770.01	-359.03
1	3	1003.8	595.35	1516.6	2074.8
2	3	463.04	-105.87	382.16	227.04

R1 = 3.3900 R2 = 2.5735 R3 = 0.9200
Q1 = 2.910 Q2 = 2.336 Q3 = 1.400

MEAN DEV. BETWEEN CALC. AND EXP. CONC. IN MOLE PCT

UNIQUAC (SPECIFIC PARAMETERS)	0.46
NRTL (SPECIFIC PARAMETERS)	0.55
UNIQUAC (COMMON PARAMETERS)	0.92





CCl_4-C_3H_6O

(1) CCL4 METHANE,TETRACHLORO

(2) C3H6O2 PROPANOIC ACID

(3) H2O WATER

IGUCHI A., FUSE K.
KAGAKU KOGAKU 36(1972)673

TEMPERATURE = 25.0 DEG C TYPE OF SYSTEM = 1

EXPERIMENTAL TIE LINES IN MOLE PCT (GRAPH.INTERPOL.)

LEFT PHASE			RIGHT PHASE		
(1)	(2)	(3)	(1)	(2)	(3)
95.776	4.224	0.0	0.025	1.956	98.019
90.560	9.440	0.0	0.052	3.344	96.604
79.417	19.822	0.760	0.083	5.835	94.081
74.040	25.223	0.737	0.102	7.426	92.473
65.831	32.772	1.397	0.126	10.781	89.093
59.635	38.358	2.007	0.291	14.144	85.564
54.619	42.801	2.580	0.731	18.866	80.403
50.533	45.727	3.740	1.205	21.934	76.861
41.068	48.294	10.638	3.246	28.520	68.234
16.331	41.941	41.729	10.192	37.651	52.157

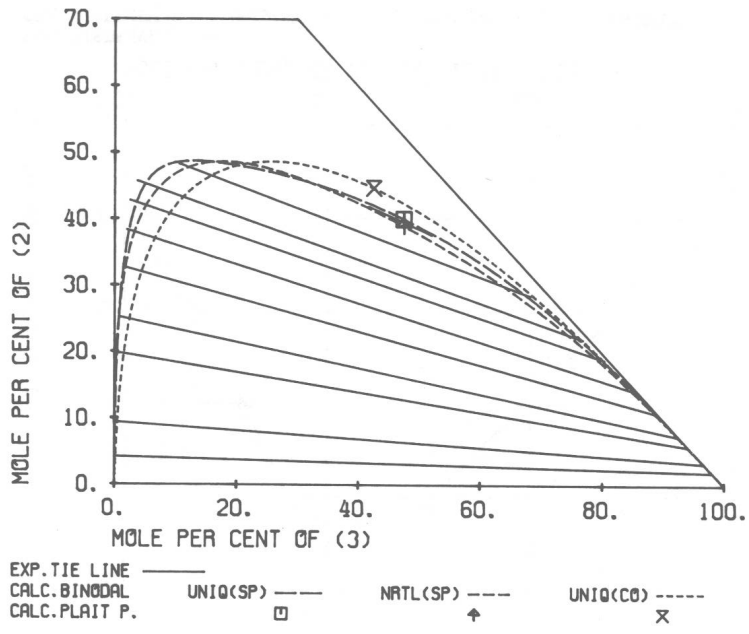
SPECIFIC MODEL PARAMETERS IN KELVIN

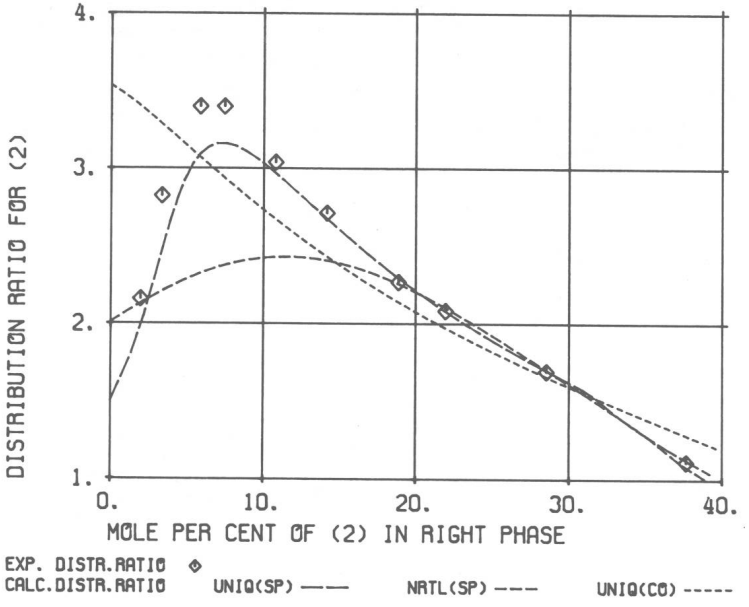
	UNIQUAC		NRTL(ALPHA=.2)	
I J	AIJ	AJI	AIJ	AJI
1 2	525.16	-250.92	693.53	-405.96
1 3	1470.0	1021.2	2588.4	2152.5
2 3	810.88	-225.50	361.86	86.533

R1 = 3.3900 R2 = 2.8768 R3 = 0.9200
Q1 = 2.910 Q2 = 2.612 Q3 = 1.400

MEAN DEV. BETWEEN CALC. AND EXP. CONC. IN MOLE PCT

UNIQUAC (SPECIFIC PARAMETERS)	0.41
NRTL (SPECIFIC PARAMETERS)	1.42
UNIQUAC (COMMON PARAMETERS)	2.20





(1) CCL4 METHANE,TETRACHLORO

(2) C3H8O 1-PROPANOL

(3) H2O WATER

DENZLER C.G.
J.PHYS.CHEM. 49(1945)358

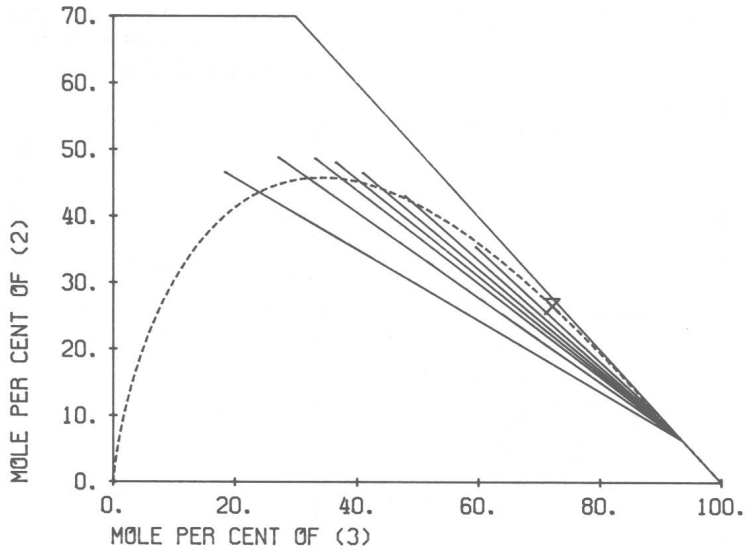
TEMPERATURE = 20.0 DEG C TYPE OF SYSTEM = 1

EXPERIMENTAL TIE LINES IN MOLE PCT

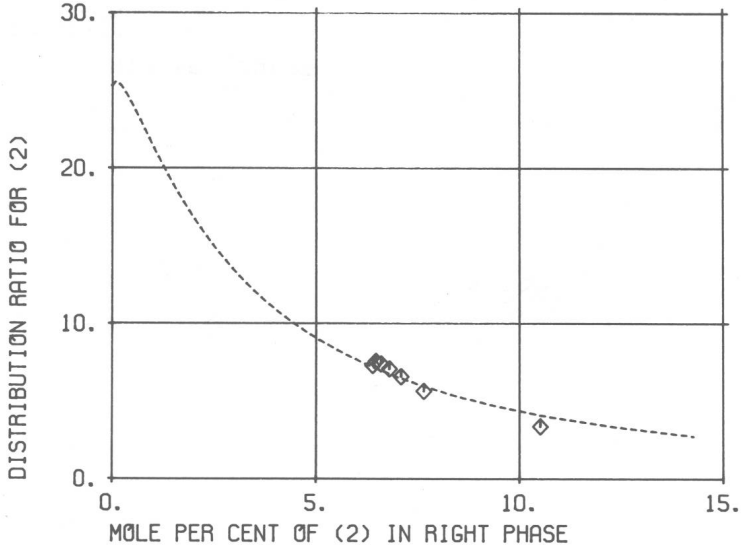
LEFT PHASE			RIGHT PHASE		
(1)	(2)	(3)	(1)	(2)	(3)
34.977	46.594	18.429	0.035	6.387	93.578
23.937	48.838	27.225	0.038	6.467	93.495
18.077	48.672	33.251	0.041	6.588	93.371
15.260	48.075	36.665	0.052	6.795	93.153
12.383	46.534	41.083	0.059	7.083	92.858
8.948	43.065	47.987	0.100	7.643	92.257
4.948	35.416	59.636	0.327	10.507	89.166

MEAN DEV. BETWEEN CALC. AND EXP. CONC. IN MOLE PCT

UNIQUAC (COMMON PARAMETERS) 2.01



EXP.TIE LINE ———
CALC.BINODAL UNIQ(CO) -----
CALC.PLAIT P. ⧖



EXP. DISTR.RATIO ◇
CALC.DISTR.RATIO UNIQ(CO) -----

CCl_4-C_3H_8O

(1) CCL4	METHANE,TETRACHLORO	
(2) C3H8O	2-PROPANOL	
(3) H2O	WATER	

IZMAILOV N.A., FRANKE A.K.
ZH.FIZ.KHIM. 29(1955)263

TEMPERATURE = 25.0 DEG C TYPE OF SYSTEM = 1

EXPERIMENTAL TIE LINES IN MOLE PCT

LEFT PHASE (1)	(2)	(3)	RIGHT PHASE (1)	(2)	(3)
98.479	1.521	0.0	0.013	3.681	96.306
96.005	3.995	0.0	0.026	5.373	94.601
89.635	9.567	0.798	0.041	6.749	93.210
70.749	23.740	5.511	0.114	8.896	90.990
56.812	31.166	12.022	0.160	9.869	89.970
43.737	37.152	19.111	0.207	10.649	89.144
33.492	39.782	26.726	0.302	11.446	88.252
19.658	39.488	40.855	0.486	12.916	86.598
14.461	37.273	48.266	0.755	14.742	84.503

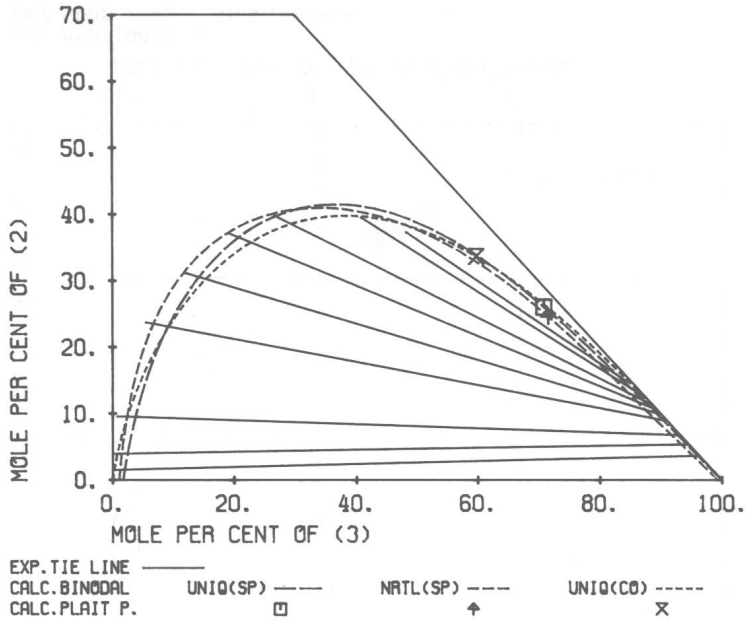
SPECIFIC MODEL PARAMETERS IN KELVIN

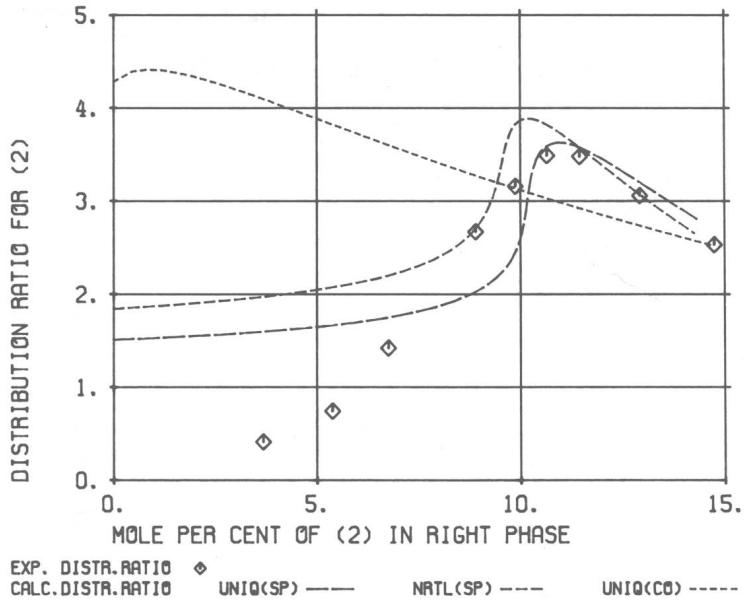
I J	UNIQUAC AIJ	UNIQUAC AJI	NRTL(ALPHA=.2) AIJ	NRTL(ALPHA=.2) AJI
1 2	336.80	-85.423	703.29	-183.39
1 3	656.78	248.47	385.90	983.89
2 3	76.985	68.463	-244.79	964.61

R1 = 3.3900 R2 = 2.7791 R3 = 0.9200
Q1 = 2.910 Q2 = 2.508 Q3 = 1.400

MEAN DEV. BETWEEN CALC. AND EXP. CONC. IN MOLE PCT

UNIQUAC (SPECIFIC PARAMETERS)	1.38
NRTL (SPECIFIC PARAMETERS)	1.21
UNIQUAC (COMMON PARAMETERS)	3.38





(1) CCL4 METHANE,TETRACHLORO

(2) C5H4O2 FURFURAL

(3) H2O WATER

KRUPATKIN I.L., GLAGOLEVA M.F.
ZH.PRIKL.KHIM.(LENINGRAD) 42(1969)1526

TEMPERATURE = 25.0 DEG C TYPE OF SYSTEM = 2

EXPERIMENTAL TIE LINES IN MOLE PCT

LEFT PHASE			RIGHT PHASE		
(1)	(2)	(3)	(1)	(2)	(3)
75.060	23.786	1.153	0.074	0.942	98.985
53.271	43.284	3.446	0.087	1.149	98.765
30.726	59.820	9.454	0.075	1.283	98.642
21.075	66.856	12.070	0.037	1.459	98.504
5.286	73.991	20.723	0.013	1.627	98.360
12.830	73.283	13.887	0.025	1.758	98.216

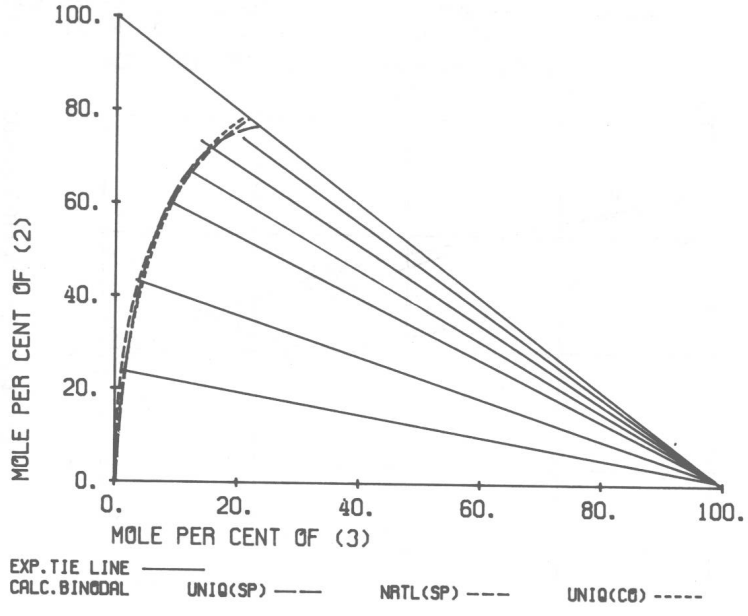
SPECIFIC MODEL PARAMETERS IN KELVIN

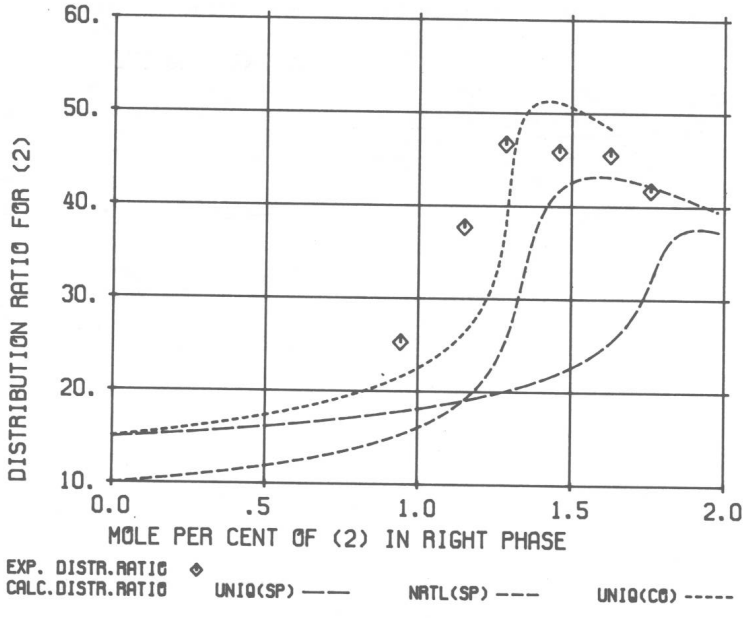
	UNIQUAC		NRTL(ALPHA=.2)	
I J	AIJ	AJI	AIJ	AJI
1 2	39.512	144.99	427.61	103.56
1 3	918.49	633.38	1527.6	1577.5
2 3	210.12	60.877	48.559	1164.6

R1 = 3.3900 R2 = 3.1680 R3 = 0.9200
Q1 = 2.910 Q2 = 2.484 Q3 = 1.400

MEAN DEV. BETWEEN CALC. AND EXP. CONC. IN MOLE PCT

UNIQUAC (SPECIFIC PARAMETERS)	0.55
NRTL (SPECIFIC PARAMETERS)	0.59
UNIQUAC (COMMON PARAMETERS)	0.65





CCl_4-$C_5H_4O_2$