JOURNAL OF CHEMICAL & ENGINEERING DATA

ARTICLE

pubs.acs.org/jced

Vapor−Liquid Equilibrium for Thiophene + Butane, + *trans*-But-2-ene, + 2-Methylpropane, and + 2-Methylpropene

Petri Uusi-Kyyny,* Juha-Pekka Pokki, Erlin Sapei, Minna Pakkanen, and Ville Alopaeus

School of Science and Technology, Research Group of Chemical Engineering, Aalto University, P.O. Box 16100, FI-00076 Aalto, Finland

ABSTRACT: The isothermal vapor−liquid equilibrium (VLE) of binary systems of thiophene + butane, + *trans*-but-2-ene, + 2-methylpropane, and + 2-methylpropene was measured at (308 and 336) K with a static total pressure apparatus. The measured data (temperature, pressure, and amounts of moles) were reduced to phase equilibrium data with Barker's method. All binary systems exhibited a positive deviation from Raoult's law.

INTRODUCTION

The sulfur content in liquid fuels is stringently regulated by legislation to reduce air pollution. One of the major components contributing to the sulfur content in liquid fuels is thiophene.[1] It is important to know the phase behavior of organic sulfur components to be able to control the sulfur content of process streams. Process streams originating from the fluid catalytic cracker (FCC) unit contribute to a large extent of the sulfur in gasoline. One processing example of such a stream is the etherification of a C4-alkane and -alkene containing process stream. The etherification unit decreases the alkene content and product vapor pressure, increases octane number of the fuel, and is one method to introduce bioethanol to the gasoline pool.[2] A substantially larger amount of C4-alkanes can be blended into the gasoline as light components by the utilization of ethers, without compromising gasoline vapor pressure specifications.

The distribution of the sulfur species is of importance not only for determining the optimal size of adsorbent beds for the removal of sulfur and oxygenate species from the nonreacted C4 fraction but also for the sulfur content of the ether product stream.

The target of this work was to measure previously unavailable vapor−liquid equilibrium (VLE) data for thiophene with C4 hydrocarbons. The measurements were made for the systems thiophene + butane, + *trans*-but-2-ene, + 2-methylpropane, and + 2-methylpropene was measured at (308 and 336) K.

EXPERIMENTAL SECTION

Materials. The suppliers and the purities of the materials used are presented in Table 1. Thiophene was analyzed with a gas chromatograph (GC), equipped with a flame ionization detector. The purity of thiophene was higher than 0.999 in mass fraction according to the GC analysis. The thiophene was dried over molecule sieves (Merck, 3A). The water content of dried thiophene was analyzed with Karl Fischer titration; it was less than $3 \cdot 10^{-5}$ in mass fraction. The degassing of thiophene was performed by vacuum rectification[3] with modifications.[4] The success of the purification was determined by comparing the measured vapor pressure and the refractive index with values obtained from the literature. Vapor pressures are shown in Table 2. Each reported pure component vapor pressure value was separately measured in separate VLE runs. The measured

Table 1. Supplier and the Purity of the Material

compound	company	mass fraction purity
butane	Messer Finland Oy	0.998
2-methylpropane	Riedel-de Haën	0.998
2-methylpropene	Riedel-de Haën	0.998
trans-but-2-ene	Fluka	> 0.998
thiophene	Merck	0.998

Table 2. Pure Compound Vapor Pressure, *P*, at Temperature *T*

compound	*T*/K	*P*/kPa	*P*/kPa		
			ref 15	ref 16	ref 17
butane	308.15	328.8	329.2	329.0	328.9
	335.60	679.3	679.3	678.1	678.2
2-methylpropane	308.14	467.4	461.9	468.1	465.8
	335.83	926.6	918.3	925.7	924.9
2-methylpropene	308.13	413.7	404.6	411.3	407.0
	336.84	855.5	847.0	857.7	849.0
trans-but-2-ene	308.14	317.3		317.3	317.3
	335.86	666.1		667.9	667.3
thiophene	308.14	17.1	16.7	16.6	16.6
	335.84	49.6	49.8	49.8	49.7
	308.15	17.1	16.7	16.7	16.6
	335.61	49.7	49.4	49.4	49.3
	308.12	16.7	16.7	16.6	16.6
	336.83	51.2	51.6	51.6	51.5
	308.13	16.5	16.7	16.6	16.6
	335.87	49.6	49.8	49.9	49.8

Received: December 22, 2010
Accepted: January 27, 2011
Published: February 18, 2011

refractive index of thiophene was 1.52869 in comparison to a literature value of 1.5287 at 293.15 K.[5] Alkanes and alkenes were degassed in the syringe pump before use by opening the vacuum valve 10 times for a period of 10 s.

Table 3. Pure Compound Physical Properties[17]

compound[a]	thiophene	butane	2-methyl-propane	2-methyl-propene	*trans*-but-2-ene
CAS	110-02-1	106-97-8	75-28-5	115-11-7	624-64-6
T_C/K	579.35	425.12	407.8	417.9	428.6
p_C/MPa	5.69	3.80	3.60	4.00	4.10
ω	0.196972	0.200164	0.183521	0.19484	0.217592
v_i/cm^3·mol^{-1}	79.4848	101.394	105.35	95.3646	93.6136

[a] Critical temperature, T_C; critical pressure, p_C; acentric factor, ω; molar volume v_i at 298 K.

Table 4. Experimental Uncertainties Used in the Error Estimate

variable	uncertainty
density correlation butane	0.3 %
density correlation 2-methylpropane	0.28 %
density correlation 2-methylpropene	0.15 %
density correlation *trans*-but-2-ene	0.76 %
density correlation thiophene	0.06 %
pump injection volume	0.02 cm^3
pump temperature	0.1 K
pump pressure	20 kPa
cell temperature	0.03 K
cell pressure	0.4 kPa

Apparatus. The static total pressure apparatus employed in the experiment has been described in detail by Uusi-Kyyny et al.[6] Temperatures were measured with Pt-100 probes connected to a temperature meter (Termolyzer S2541, Frontek). Probes had been calibrated at the Centre for Metrology and Accreditation, Finland. The pressure of the cell was measured with a Digiquartz 2300A-101-CE pressure transducer connected to a Digiquartz 740 intelligent display unit (Paroscientific). The range of the pressure measurement was from (0 to 2070) kPa with a temperature range from (219 to 380) K. The equilibrium cell had a total volume of 103.3 cm^3 with an uncertainty of 0.02 cm^3. The cell volume had been determined by injecting degassed water in the cell at 298.15 K. Injections of the compounds were made with syringe pumps (ISCO 260D and 100D).

Procedure. After degassing, the first compound was injected into the cell, and the pure compound vapor pressure was measured and compared to the value obtained from the literature. If the error was within an acceptable limit, the second compound was added into the cell, and after the cell content had reached equilibrium (approximately 20 min), the total pressure was measured. The addition of the second compound was repeated until an approximately equimolar composition was reached. At this point, the cell was drained and emptied with a vacuum. Then the injection of the compounds was repeated in a reversed order to obtain the other half of the data set. The quality of the data was evaluated based on how well the vapor pressures of each half set coincided at the equimolar composition and how well the measured pure component vapor pressure agreed with the values reported in the literature.

Data Reduction. The data measured in the experiment consisted of the total pressure, temperature, and the total composition inside the cell at equilibrium. To obtain the compositions of the vapor and liquid phases, the data were

Table 5. Experimental Temperature, T; Legendre Liquid Activity Coefficient Model Parameters, Legendre, $a_{i,i}$; Absolute Average Pressure Residuals, $|\Delta P|$; Infinite Dilution Activity Coefficients γ_i^∞; Wilson Liquid Activity Coefficient Model Parameters, Wilson $\lambda_{i,j}$ for System 1 (Butane + Thiophene), System 2 (2-Methylpropane + Thiophene), System 3 (2-Methylpropene + Thiophene), and System 4 (*trans*-But-2-ene + Thiophene)

system	1	2	3	4
T/K	308	308	308	308
Legendre, $a_{0,0}$	1.03164	1.14818	0.741557	0.700856
Legendre, $a_{1,0}$	−0.06337	−0.0651646	0.022106	−0.012097
Legendre, $a_{2,0}$	0.014503	0.018914	0.015157	0.006789
Legendre, $a_{3,0}$	−0.00794	−0.00660089	−0.019623	
$\|\Delta P\|$/kPa	0.07	0.1	0.5	0.1
Legendre γ_1^∞, γ_2^∞	3.06, 2.65	3.45, 2.99	2.13, 2.14	2.05, 2.00
T/K	336	336	337	336
Legendre, $a_{0,0}$	0.896413	1.02483	0.654009	0.625123
Legendre, $a_{1,0}$	−0.0527467	−0.0533314	−0.000239	−0.014374
Legendre, $a_{2,0}$	0.0135124	0.0162851	0.008726	0.005222
Legendre, $a_{3,0}$	−0.00143523	−0.00218268	−0.006205	
$\|\Delta P\|$/kPa	0.2	0.1	0.3	0.2
Legendre γ_1^∞, γ_2^∞	2.62, 2.36	2.99, 2.63	1.95, 1.90	1.91, 1.83
T/K	308, 336	308, 336	308, 337	308, 336
Wilson $\lambda_{1,2}$/K	155.876	168.750	51.8016	82.7176
Wilson $\lambda_{2,1}$/K	214.395	250.108	193.786	154.673
$\|\Delta P\|$/kPa	1.9	1.6	1.2	0.7
γ_1^∞, γ_2^∞, Wilson, T = 308 K	3.04, 2.66	3.46, 2.99	2.04, 2.10	2.05, 1.99
γ_1^∞, γ_2^∞, Wilson, T = 336 K	2.81, 2.47	3.17, 2.74	1.94, 1.97	1.95, 1.88

Table 6. VLE Data for Butane (1) + Thiophene (2)[a]

T/K	n_1/mol	n_2/mol	z_1	p_{measd}/kPa	p_{Leg}/kPa	x_1	y_1	γ_1	γ_2
308.15 ± 0.03	0.4561 ± 0.0049	0.0000 ± 0.0000	1.0000 ± 0.0000	328.8 ± 0.4	328.8 ± 0.6	1.0000 ± 0.0007	1.0000 ± 0.0002	1.00 ± 0.00	2.65 ± 0.09
308.15 ± 0.03	0.4561 ± 0.0049	0.0039 ± 0.0003	0.9914 ± 0.0007	326.0 ± 0.4	326.1 ± 0.7	0.9913 ± 0.0012	0.9987 ± 0.0004	1.00 ± 0.00	2.62 ± 0.08
308.15 ± 0.03	0.4561 ± 0.0049	0.0144 ± 0.0004	0.9695 ± 0.0012	319.4 ± 0.4	319.5 ± 0.7	0.9691 ± 0.0015	0.9953 ± 0.0006	1.00 ± 0.00	2.52 ± 0.06
308.15 ± 0.03	0.4561 ± 0.0049	0.0239 ± 0.0005	0.9502 ± 0.0015	313.9 ± 0.4	313.9 ± 0.7	0.9496 ± 0.0024	0.9925 ± 0.0009	1.00 ± 0.00	2.44 ± 0.04
308.15 ± 0.03	0.4561 ± 0.0049	0.0506 ± 0.0008	0.9002 ± 0.0023	300.1 ± 0.4	300.1 ± 0.7	0.8990 ± 0.0031	0.9856 ± 0.0011	1.01 ± 0.00	2.24 ± 0.02
308.15 ± 0.03	0.4561 ± 0.0049	0.0806 ± 0.0011	0.8499 ± 0.0031	287.5 ± 0.4	287.4 ± 0.6	0.8484 ± 0.0038	0.9793 ± 0.0012	1.02 ± 0.00	2.06 ± 0.01
308.15 ± 0.03	0.4561 ± 0.0049	0.1142 ± 0.0014	0.7997 ± 0.0037	275.7 ± 0.4	275.6 ± 0.5	0.7980 ± 0.0043	0.9735 ± 0.0013	1.04 ± 0.01	1.91 ± 0.01
308.15 ± 0.03	0.4561 ± 0.0049	0.1517 ± 0.0018	0.7503 ± 0.0042	264.8 ± 0.4	264.7 ± 0.4	0.7486 ± 0.0047	0.9682 ± 0.0014	1.06 ± 0.01	1.77 ± 0.01
308.16 ± 0.03	0.4561 ± 0.0049	0.1947 ± 0.0022	0.7008 ± 0.0047	254.4 ± 0.4	254.4 ± 0.5	0.6991 ± 0.0050	0.9632 ± 0.0015	1.09 ± 0.01	1.66 ± 0.00
308.16 ± 0.03	0.4561 ± 0.0049	0.2462 ± 0.0027	0.6494 ± 0.005	244.0 ± 0.4	244.1 ± 0.5	0.6478 ± 0.0052	0.9582 ± 0.0015	1.13 ± 0.01	1.55 ± 0.00
308.16 ± 0.03	0.4561 ± 0.0049	0.3045 ± 0.0033	0.5996 ± 0.0052	234.2 ± 0.4	234.4 ± 0.5	0.5982 ± 0.0054	0.9535 ± 0.0016	1.17 ± 0.01	1.46 ± 0.00
308.16 ± 0.03	0.4561 ± 0.0049	0.3727 ± 0.0040	0.5503 ± 0.0053	224.6 ± 0.4	224.7 ± 0.5	0.5491 ± 0.0054	0.9487 ± 0.0017	1.22 ± 0.01	1.38 ± 0.00
308.15 ± 0.03	0.4582 ± 0.0049	0.4581 ± 0.0049	0.5001 ± 0.0053	215.0 ± 0.4	214.8 ± 0.5	0.4992 ± 0.0054	0.9437 ± 0.0017	1.28 ± 0.01	1.31 ± 0.00
308.16 ± 0.03	0.4561 ± 0.0049	0.4548 ± 0.0049	0.5007 ± 0.0053	214.9 ± 0.4	214.9 ± 0.5	0.4998 ± 0.0053	0.9437 ± 0.0019	1.28 ± 0.02	1.31 ± 0.00
308.15 ± 0.03	0.3744 ± 0.0040	0.4581 ± 0.0049	0.4497 ± 0.0053	204.2 ± 0.4	204.2 ± 0.4	0.4483 ± 0.0052	0.9381 ± 0.0020	1.35 ± 0.02	1.25 ± 0.00
308.15 ± 0.03	0.3026 ± 0.0033	0.4581 ± 0.0049	0.3978 ± 0.0052	192.5 ± 0.4	192.5 ± 0.4	0.3958 ± 0.0050	0.9316 ± 0.0022	1.43 ± 0.02	1.19 ± 0.00
308.15 ± 0.03	0.2453 ± 0.0027	0.4581 ± 0.0049	0.3487 ± 0.005	180.4 ± 0.4	180.4 ± 0.5	0.3462 ± 0.0046	0.9243 ± 0.0024	1.53 ± 0.03	1.15 ± 0.00
308.15 ± 0.03	0.1950 ± 0.0022	0.4581 ± 0.0049	0.2986 ± 0.0046	166.8 ± 0.4	166.7 ± 0.5	0.2956 ± 0.0042	0.9152 ± 0.0026	1.65 ± 0.03	1.11 ± 0.00
308.15 ± 0.03	0.1521 ± 0.0018	0.4581 ± 0.0049	0.2492 ± 0.0042	151.4 ± 0.4	151.4 ± 0.4	0.2458 ± 0.0036	0.9035 ± 0.0028	1.78 ± 0.04	1.07 ± 0.00
308.15 ± 0.03	0.1146 ± 0.0014	0.4581 ± 0.0049	0.2001 ± 0.0037	133.8 ± 0.4	133.8 ± 0.5	0.1966 ± 0.0030	0.8873 ± 0.0032	1.94 ± 0.05	1.05 ± 0.00
308.15 ± 0.03	0.0809 ± 0.0010	0.4581 ± 0.0049	0.1501 ± 0.003	112.5 ± 0.4	112.6 ± 0.6	0.1466 ± 0.0022	0.8617 ± 0.0039	2.14 ± 0.06	1.03 ± 0.00
308.15 ± 0.03	0.0513 ± 0.0007	0.4581 ± 0.0049	0.1008 ± 0.0023	87.4 ± 0.4	87.4 ± 0.5	0.0977 ± 0.0014	0.8163 ± 0.0059	2.38 ± 0.08	1.01 ± 0.00
308.15 ± 0.03	0.0249 ± 0.0005	0.4581 ± 0.0049	0.0515 ± 0.0014	56.7 ± 0.4	56.8 ± 0.6	0.0495 ± 0.0010	0.7084 ± 0.0079	2.67 ± 0.09	1.00 ± 0.00
308.15 ± 0.03	0.0150 ± 0.0004	0.4581 ± 0.0049	0.0317 ± 0.0011	42.7 ± 0.4	42.6 ± 0.7	0.0304 ± 0.0007	0.6063 ± 0.0132	2.81 ± 0.10	1.00 ± 0.00
308.15 ± 0.03	0.0054 ± 0.0003	0.4581 ± 0.0049	0.0117 ± 0.0007	27.1 ± 0.4	26.9 ± 0.4	0.0112 ± 0.0000	0.3699 ± 0.0000	2.96 ± 0.10	1.00 ± 0.00
308.15 ± 0.03	0.0000 ± 0.0000	0.4581 ± 0.0049	0.0000 ± 0.0000	17.1 ± 0.4	17.1 ± 0	0.0000 ± 0.0000	0.0000 ± 0.0000	3.05 ± 0.00	1.00 ± 0.00
335.60 ± 0.03	0.4445 ± 0.0048	0.0000 ± 0.0000	1.0000 ± 0.0000	677.9 ± 0.4	677.9 ± 0.4	1.0000 ± 0.0000	1.0000 ± 0.0000	1.00 ± 0.00	2.36 ± 0.08
335.61 ± 0.03	0.4445 ± 0.0048	0.0048 ± 0.0003	0.9892 ± 0.0008	671.3 ± 0.4	670.9 ± 0.8	0.9889 ± 0.0008	0.9977 ± 0.0003	1.00 ± 0.00	2.31 ± 0.07
335.61 ± 0.03	0.4445 ± 0.0048	0.0139 ± 0.0004	0.9698 ± 0.0012	659.1 ± 0.4	658.6 ± 0.9	0.9690 ± 0.0012	0.9936 ± 0.0005	1.00 ± 0.00	2.24 ± 0.06
335.61 ± 0.03	0.4445 ± 0.0048	0.0233 ± 0.0005	0.9503 ± 0.0015	647.2 ± 0.4	646.5 ± 0.9	0.9490 ± 0.0016	0.9896 ± 0.0006	1.00 ± 0.00	2.17 ± 0.05
335.62 ± 0.03	0.4445 ± 0.0048	0.0497 ± 0.0008	0.8994 ± 0.0024	617.1 ± 0.4	616.8 ± 0.9	0.8973 ± 0.0025	0.9799 ± 0.0010	1.01 ± 0.00	2.01 ± 0.04
335.62 ± 0.03	0.4445 ± 0.0048	0.0792 ± 0.0011	0.8488 ± 0.0031	589.3 ± 0.4	589.2 ± 0.8	0.8460 ± 0.0032	0.9710 ± 0.0011	1.02 ± 0.00	1.87 ± 0.02
335.61 ± 0.03	0.4445 ± 0.0048	0.1115 ± 0.0014	0.7995 ± 0.0037	563.9 ± 0.4	564.0 ± 0.7	0.7964 ± 0.0038	0.9629 ± 0.0012	1.03 ± 0.00	1.75 ± 0.01
335.62 ± 0.03	0.4445 ± 0.0048	0.1486 ± 0.0018	0.7495 ± 0.0043	539.7 ± 0.4	539.8 ± 0.6	0.7462 ± 0.0044	0.9550 ± 0.0013	1.05 ± 0.01	1.64 ± 0.01
335.62 ± 0.03	0.4445 ± 0.0048	0.1904 ± 0.0022	0.7001 ± 0.0047	516.9 ± 0.4	517.0 ± 0.5	0.6969 ± 0.0048	0.9475 ± 0.0013	1.08 ± 0.01	1.54 ± 0.00
335.62 ± 0.03	0.4445 ± 0.0048	0.2410 ± 0.0027	0.6485 ± 0.0050	493.8 ± 0.4	493.8 ± 0.5	0.6455 ± 0.0051	0.9398 ± 0.0013	1.11 ± 0.01	1.46 ± 0.00
335.62 ± 0.03	0.4445 ± 0.0048	0.2968 ± 0.0033	0.5997 ± 0.0052	472.3 ± 0.4	472.3 ± 0.6	0.5971 ± 0.0053	0.9325 ± 0.0014	1.14 ± 0.01	1.39 ± 0.00
335.61 ± 0.03	0.4445 ± 0.0048	0.3643 ± 0.0039	0.5496 ± 0.0053	450.6 ± 0.4	450.4 ± 0.6	0.5476 ± 0.0054	0.9248 ± 0.0014	1.19 ± 0.01	1.32 ± 0.00
335.61 ± 0.03	0.4445 ± 0.0048	0.4443 ± 0.0048	0.5001 ± 0.0054	429.0 ± 0.4	428.5 ± 0.6	0.4987 ± 0.0054	0.9168 ± 0.0015	1.23 ± 0.01	1.26 ± 0.00
335.61 ± 0.03	0.4442 ± 0.0048	0.4484 ± 0.0048	0.4976 ± 0.0054	427.2 ± 0.4	427.4 ± 0.6	0.4963 ± 0.0054	0.9164 ± 0.0015	1.24 ± 0.01	1.26 ± 0.00
335.62 ± 0.03	0.3633 ± 0.0039	0.4484 ± 0.0048	0.4476 ± 0.0053	403.6 ± 0.4	403.8 ± 0.6	0.4452 ± 0.0053	0.9074 ± 0.0016	1.30 ± 0.01	1.21 ± 0.00
335.61 ± 0.03	0.2958 ± 0.0032	0.4484 ± 0.0048	0.3975 ± 0.0052	378.9 ± 0.4	379.0 ± 0.5	0.3941 ± 0.0052	0.8971 ± 0.0017	1.37 ± 0.02	1.16 ± 0.00
335.62 ± 0.03	0.2394 ± 0.0027	0.4484 ± 0.0048	0.3481 ± 0.0050	352.9 ± 0.4	352.9 ± 0.6	0.3438 ± 0.0050	0.8853 ± 0.0018	1.45 ± 0.02	1.12 ± 0.00
335.62 ± 0.03	0.1905 ± 0.0022	0.4484 ± 0.0048	0.2982 ± 0.0046	324.3 ± 0.4	324.2 ± 0.6	0.2930 ± 0.0046	0.8708 ± 0.0019	1.55 ± 0.02	1.09 ± 0.00
335.61 ± 0.03	0.1492 ± 0.0017	0.4484 ± 0.0048	0.2496 ± 0.0042	293.3 ± 0.4	293.3 ± 0.5	0.2439 ± 0.0042	0.8526 ± 0.0019	1.66 ± 0.03	1.06 ± 0.00
335.61 ± 0.03	0.1118 ± 0.0013	0.4484 ± 0.0048	0.1995 ± 0.0037	257.3 ± 0.4	257.3 ± 0.5	0.1935 ± 0.0036	0.8268 ± 0.0020	1.79 ± 0.03	1.04 ± 0.00
335.61 ± 0.03	0.0797 ± 0.0010	0.4484 ± 0.0048	0.1509 ± 0.0030	217.5 ± 0.4	217.6 ± 0.5	0.1451 ± 0.0030	0.7892 ± 0.0020	1.95 ± 0.04	1.02 ± 0.00
335.61 ± 0.03	0.0505 ± 0.0007	0.4484 ± 0.0048	0.1012 ± 0.0023	170.7 ± 0.4	170.7 ± 0.6	0.0964 ± 0.0022	0.7237 ± 0.0021	2.13 ± 0.05	1.01 ± 0.00
335.60 ± 0.03	0.0242 ± 0.0004	0.4484 ± 0.0048	0.0513 ± 0.0014	115.8 ± 0.4	115.8 ± 0.4	0.0482 ± 0.0014	0.5817 ± 0.0026	2.35 ± 0.07	1.00 ± 0.00
335.60 ± 0.03	0.0146 ± 0.0004	0.4484 ± 0.0048	0.0315 ± 0.0011	91.6 ± 0.4	91.6 ± 0.6	0.0295 ± 0.0010	0.4655 ± 0.0036	2.45 ± 0.08	1.00 ± 0.00
335.60 ± 0.03	0.0051 ± 0.0003	0.4484 ± 0.0048	0.0113 ± 0.0007	65.1 ± 0.4	65.2 ± 0.8	0.0105 ± 0.0007	0.2420 ± 0.0071	2.56 ± 0.08	1.00 ± 0.00
335.61 ± 0.03	0.0000 ± 0.0000	0.4484 ± 0.0048	0.0000 ± 0.0000	49.7 ± 0.4	49.7 ± 0.4	0.0000 ± 0.0000	0.0000 ± 0.0000	2.62 ± 0.09	1.00 ± 0.00

[a] Experimental temperature T; amount of component in the equilibrium cell n_i; total mole fraction z_1; experimental pressure p_{measd}; pressure calculated from the Legendre polynomial fit p_{Leg}; liquid and vapor phase equilibrium mole fractions x_1 and y_1; activity coefficients γ_1 and γ_2.

dx.doi.org/10.1021/je101343m |J. Chem. Eng. Data 2011, 56, 614–621

Table 7. VLE Data for 2-Methylpropane (1) + Thiophene (2)[a]

T/K	n_1/mol	n_2/mol	z_1	p_{measd}/kPa	p_{Leg}/kPa	x_1	y_1	γ_1	γ_2
308.14 ± 0.03	0.4423 ± 0.0047	0.0000 ± 0.0000	1.0000 ± 0.0000	467.4 ± 0.4	467.4 ± 0.4	1.000 ± 0.0000	1.0000 ± 0.0000	1.00 ± 0.00	2.99 ± 0.11
308.15 ± 0.03	0.4423 ± 0.0047	0.0036 ± 0.0003	0.9920 ± 0.0007	463.4 ± 0.4	463.7 ± 0.7	0.9918 ± 0.0008	0.9989 ± 0.0002	1.00 ± 0.00	2.94 ± 0.10
308.15 ± 0.03	0.4423 ± 0.0047	0.0140 ± 0.0004	0.9693 ± 0.0012	453.2 ± 0.4	453.3 ± 0.8	0.9687 ± 0.0012	0.9960 ± 0.0003	1.00 ± 0.00	2.81 ± 0.08
308.15 ± 0.03	0.4423 ± 0.0047	0.0234 ± 0.0005	0.9497 ± 0.0015	444.6 ± 0.4	444.7 ± 0.9	0.9487 ± 0.0016	0.9937 ± 0.0005	1.00 ± 0.00	2.70 ± 0.07
308.15 ± 0.03	0.4423 ± 0.0047	0.0501 ± 0.0008	0.8982 ± 0.0024	423.5 ± 0.4	423.6 ± 0.9	0.8964 ± 0.0025	0.9880 ± 0.0007	1.01 ± 0.00	2.44 ± 0.04
308.15 ± 0.03	0.4423 ± 0.0047	0.0789 ± 0.0011	0.8487 ± 0.0031	405.3 ± 0.4	405.4 ± 0.9	0.8464 ± 0.0032	0.9831 ± 0.0009	1.02 ± 0.00	2.23 ± 0.02
308.15 ± 0.03	0.4423 ± 0.0047	0.1103 ± 0.0014	0.8004 ± 0.0037	389.1 ± 0.4	389.1 ± 0.8	0.7978 ± 0.0038	0.9789 ± 0.0010	1.04 ± 0.00	2.05 ± 0.01
308.15 ± 0.03	0.4423 ± 0.0047	0.1474 ± 0.0017	0.7500 ± 0.0043	373.4 ± 0.4	373.4 ± 0.6	0.7473 ± 0.0043	0.9748 ± 0.0011	1.07 ± 0.01	1.89 ± 0.01
308.15 ± 0.03	0.4423 ± 0.0047	0.1899 ± 0.0022	0.6996 ± 0.0047	358.7 ± 0.4	358.8 ± 0.5	0.6969 ± 0.0048	0.9711 ± 0.0011	1.10 ± 0.01	1.74 ± 0.00
308.14 ± 0.03	0.4423 ± 0.0047	0.2380 ± 0.0027	0.6502 ± 0.0050	345.1 ± 0.4	345.1 ± 0.5	0.6476 ± 0.0051	0.9677 ± 0.0012	1.14 ± 0.01	1.62 ± 0.00
308.14 ± 0.03	0.4423 ± 0.0047	0.2932 ± 0.0032	0.6014 ± 0.0052	332.1 ± 0.4	332.1 ± 0.6	0.5991 ± 0.0053	0.9645 ± 0.0012	1.19 ± 0.01	1.52 ± 0.00
308.14 ± 0.03	0.4423 ± 0.0047	0.3596 ± 0.0039	0.5516 ± 0.0053	319.1 ± 0.4	319.0 ± 0.6	0.5497 ± 0.0054	0.9612 ± 0.0013	1.24 ± 0.01	1.43 ± 0.00
308.14 ± 0.03	0.4423 ± 0.0047	0.4398 ± 0.0047	0.5014 ± 0.0054	305.8 ± 0.4	305.7 ± 0.5	0.5000 ± 0.0054	0.9577 ± 0.0013	1.31 ± 0.01	1.35 ± 0.00
308.15 ± 0.03	0.4409 ± 0.0047	0.4410 ± 0.0047	0.4999 ± 0.0054	305.5 ± 0.4	305.4 ± 0.5	0.4986 ± 0.0054	0.9576 ± 0.0013	1.31 ± 0.01	1.35 ± 0.00
308.15 ± 0.03	0.3608 ± 0.0039	0.4410 ± 0.0047	0.4500 ± 0.0053	291.2 ± 0.4	291.2 ± 0.4	0.4478 ± 0.0054	0.9539 ± 0.0014	1.39 ± 0.02	1.28 ± 0.00
308.15 ± 0.03	0.2953 ± 0.0032	0.4410 ± 0.0047	0.4011 ± 0.0052	276.2 ± 0.4	276.3 ± 0.5	0.3979 ± 0.0052	0.9498 ± 0.0015	1.49 ± 0.02	1.22 ± 0.00
308.15 ± 0.03	0.2404 ± 0.0027	0.4410 ± 0.0047	0.3528 ± 0.0050	260.1 ± 0.4	260.2 ± 0.6	0.3488 ± 0.0050	0.9451 ± 0.0017	1.6 ± 0.02	1.17 ± 0.00
308.14 ± 0.03	0.1914 ± 0.0022	0.4410 ± 0.0047	0.3027 ± 0.0047	241.2 ± 0.4	241.2 ± 0.6	0.2979 ± 0.0047	0.9391 ± 0.0018	1.73 ± 0.03	1.12 ± 0.00
308.14 ± 0.03	0.1489 ± 0.0017	0.4410 ± 0.0047	0.2524 ± 0.0042	219.5 ± 0.4	219.4 ± 0.5	0.2469 ± 0.0042	0.9311 ± 0.0019	1.90 ± 0.03	1.08 ± 0.00
308.14 ± 0.03	0.1132 ± 0.0014	0.4410 ± 0.0047	0.2043 ± 0.0037	194.8 ± 0.4	194.8 ± 0.4	0.1985 ± 0.0037	0.9205 ± 0.0021	2.08 ± 0.04	1.05 ± 0.00
308.14 ± 0.03	0.0807 ± 0.0010	0.4410 ± 0.0047	0.1547 ± 0.0031	164.4 ± 0.4	164.4 ± 0.6	0.1489 ± 0.0030	0.9033 ± 0.0023	2.32 ± 0.05	1.03 ± 0.00
308.14 ± 0.03	0.0533 ± 0.0007	0.4410 ± 0.0047	0.1079 ± 0.0024	129.5 ± 0.4	129.6 ± 0.7	0.1028 ± 0.0023	0.8744 ± 0.0027	2.59 ± 0.07	1.02 ± 0.00
308.15 ± 0.03	0.0271 ± 0.0005	0.4410 ± 0.0047	0.0579 ± 0.0015	83.9 ± 0.4	84.0 ± 0.6	0.0544 ± 0.0015	0.8014 ± 0.0040	2.94 ± 0.09	1.00 ± 0.00
308.15 ± 0.03	0.0173 ± 0.0004	0.4410 ± 0.0047	0.0377 ± 0.0012	62.6 ± 0.4	62.6 ± 0.5	0.0352 ± 0.0011	0.7310 ± 0.0052	3.10 ± 0.11	1.00 ± 0.00
308.15 ± 0.03	0.0084 ± 0.0003	0.4410 ± 0.0047	0.0188 ± 0.0008	40.7 ± 0.4	40.7 ± 0.7	0.0174 ± 0.0008	0.5830 ± 0.0089	3.27 ± 0.12	1.00 ± 0.00
308.14 ± 0.03	0.0000 ± 0.0000	0.4410 ± 0.0047	0.0000 ± 0.0000	17.1 ± 0.4	17.1 ± 0.4	0.0000 ± 0.0000	0.0000 ± 0.0000	3.45 ± 0.13	1.00 ± 0.00
335.83 ± 0.03	0.4224 ± 0.0045	0.0000 ± 0.0000	1.0000 ± 0.0000	926.6 ± 0.4	926.6 ± 0.4	1.0000 ± 0.0000	1.0000 ± 0.0000	1.00 ± 0.00	2.63 ± 0.10
335.83 ± 0.03	0.4224 ± 0.0045	0.0051 ± 0.0003	0.9881 ± 0.0008	914.6 ± 0.4	914.7 ± 1	0.9876 ± 0.0009	0.9976 ± 0.0003	1.00 ± 0.00	2.57 ± 0.08
335.83 ± 0.03	0.4224 ± 0.0045	0.0135 ± 0.0004	0.9690 ± 0.0012	896.6 ± 0.4	896.5 ± 1.1	0.9677 ± 0.0013	0.9940 ± 0.0004	1.00 ± 0.00	2.49 ± 0.07
335.83 ± 0.03	0.4224 ± 0.0045	0.0228 ± 0.0005	0.9488 ± 0.0016	878.0 ± 0.4	877.8 ± 1.2	0.9468 ± 0.0017	0.9903 ± 0.0006	1.00 ± 0.00	2.40 ± 0.06
335.83 ± 0.03	0.4224 ± 0.0045	0.0476 ± 0.0007	0.8987 ± 0.0024	834.8 ± 0.4	834.9 ± 1.3	0.8952 ± 0.0025	0.9820 ± 0.0008	1.01 ± 0.00	2.20 ± 0.03
335.83 ± 0.03	0.4224 ± 0.0045	0.0754 ± 0.0010	0.8486 ± 0.0031	796.0 ± 0.4	796.0 ± 1.2	0.8442 ± 0.0033	0.9745 ± 0.0010	1.02 ± 0.00	2.03 ± 0.02
335.84 ± 0.03	0.4224 ± 0.0045	0.1059 ± 0.0013	0.7995 ± 0.0038	761.0 ± 0.4	761.0 ± 1.0	0.7945 ± 0.0039	0.9679 ± 0.0010	1.04 ± 0.00	1.88 ± 0.01
335.83 ± 0.03	0.4224 ± 0.0045	0.1403 ± 0.0017	0.7507 ± 0.0043	728.3 ± 0.4	728.5 ± 0.8	0.7455 ± 0.0044	0.9618 ± 0.0011	1.06 ± 0.01	1.75 ± 0.00
335.83 ± 0.03	0.4224 ± 0.0045	0.1804 ± 0.0021	0.7007 ± 0.0047	697.1 ± 0.4	697.4 ± 0.7	0.6956 ± 0.0048	0.9560 ± 0.0011	1.09 ± 0.01	1.64 ± 0.00
335.83 ± 0.03	0.4224 ± 0.0045	0.2263 ± 0.0025	0.6511 ± 0.0050	667.7 ± 0.4	667.8 ± 0.7	0.6464 ± 0.0051	0.9504 ± 0.0011	1.13 ± 0.01	1.54 ± 0.00
335.83 ± 0.03	0.4224 ± 0.0045	0.2825 ± 0.0031	0.5992 ± 0.0052	637.9 ± 0.4	637.9 ± 0.7	0.5951 ± 0.0053	0.9447 ± 0.0011	1.17 ± 0.01	1.45 ± 0.00
335.83 ± 0.03	0.4224 ± 0.0045	0.3461 ± 0.0038	0.5496 ± 0.0054	609.6 ± 0.4	609.6 ± 0.6	0.5463 ± 0.0054	0.9392 ± 0.0011	1.22 ± 0.01	1.37 ± 0.00
335.83 ± 0.03	0.4224 ± 0.0045	0.4228 ± 0.0045	0.4998 ± 0.0054	581.1 ± 0.4	581.0 ± 0.5	0.4974 ± 0.0054	0.9335 ± 0.0012	1.28 ± 0.01	1.30 ± 0.00
335.83 ± 0.03	0.4219 ± 0.0045	0.4226 ± 0.0045	0.4996 ± 0.0054	580.9 ± 0.4	580.8 ± 0.5	0.4972 ± 0.0054	0.9334 ± 0.0012	1.28 ± 0.01	1.30 ± 0.00
335.83 ± 0.03	0.3465 ± 0.0037	0.4226 ± 0.0045	0.4505 ± 0.0053	550.3 ± 0.4	550.3 ± 0.5	0.4466 ± 0.0054	0.9271 ± 0.0012	1.35 ± 0.02	1.24 ± 0.00
335.83 ± 0.03	0.2837 ± 0.0031	0.4226 ± 0.0045	0.4016 ± 0.0052	518.2 ± 0.4	518.2 ± 0.5	0.3961 ± 0.0052	0.9199 ± 0.0012	1.43 ± 0.02	1.19 ± 0.00
335.83 ± 0.03	0.2301 ± 0.0025	0.4226 ± 0.0045	0.3525 ± 0.0050	483.4 ± 0.4	483.5 ± 0.5	0.3455 ± 0.0050	0.9116 ± 0.0013	1.53 ± 0.02	1.14 ± 0.00
335.83 ± 0.03	0.1837 ± 0.0020	0.4226 ± 0.0045	0.3030 ± 0.0046	444.9 ± 0.4	444.9 ± 0.6	0.2947 ± 0.0046	0.9013 ± 0.0014	1.64 ± 0.03	1.10 ± 0.00
335.84 ± 0.03	0.1448 ± 0.0016	0.4226 ± 0.0045	0.2551 ± 0.0042	403.2 ± 0.4	403.2 ± 0.6	0.2458 ± 0.0042	0.8884 ± 0.0014	1.78 ± 0.03	1.07 ± 0.00
335.84 ± 0.03	0.1096 ± 0.0013	0.4226 ± 0.0045	0.2059 ± 0.0037	354.6 ± 0.4	354.5 ± 0.5	0.1962 ± 0.0036	0.8701 ± 0.0015	1.94 ± 0.04	1.05 ± 0.00
335.84 ± 0.03	0.0785 ± 0.0009	0.4226 ± 0.0045	0.1567 ± 0.0030	298.2 ± 0.4	298.2 ± 0.6	0.1473 ± 0.0030	0.8423 ± 0.0016	2.13 ± 0.04	1.03 ± 0.00
335.84 ± 0.03	0.0513 ± 0.0007	0.4226 ± 0.0045	0.1083 ± 0.0023	234.1 ± 0.4	234.0 ± 0.7	0.1002 ± 0.0022	0.7952 ± 0.0018	2.35 ± 0.05	1.01 ± 0.00
335.84 ± 0.03	0.0262 ± 0.0004	0.4226 ± 0.0045	0.0584 ± 0.0014	156.8 ± 0.4	156.6 ± 0.6	0.0530 ± 0.0013	0.6886 ± 0.0025	2.62 ± 0.07	1.00 ± 0.00
335.84 ± 0.03	0.0172 ± 0.0003	0.4226 ± 0.0045	0.0392 ± 0.0011	123.5 ± 0.4	123.5 ± 0.8	0.0353 ± 0.0010	0.6028 ± 0.0036	2.73 ± 0.08	1.00 ± 0.00
335.83 ± 0.03	0.0092 ± 0.0002	0.4226 ± 0.0045	0.0212 ± 0.0007	90.6 ± 0.4	90.7 ± 0.8	0.0189 ± 0.0006	0.4560 ± 0.0047	2.85 ± 0.08	1.00 ± 0.00
335.84 ± 0.03	0.0000 ± 0.0000	0.4226 ± 0.0045	0.0000 ± 0.0000	49.6 ± 0.4	49.6 ± 0.4	0.0000 ± 0.0000	0.0000 ± 0.0000	2.99 ± 0.09	1.00 ± 0.00

[a] Experimental temperature T; amount of component in the equilibrium cell n_i; total mole fraction z_1; experimental pressure p_{measd}; pressure calculated from the Legendre polynomial fit p_{Leg}; liquid and vapor phase equilibrium mole fractions x_1 and y_1; activity coefficients γ_1 and γ_2.

dx.doi.org/10.1021/je101343m |J. Chem. Eng. Data 2011, 56, 614–621

Table 8. VLE Data for 2-Methylpropene (1) + Thiophene (2)[a]

T/K	n_1/mol	n_2/mol	z_1	p_{measd}/kPa	p_{Leg}/kPa	x_1	y_1	γ_1	γ_2
308.13 ± 0.03	0.4822 ± 0.0052	0.0000 ± 0.0000	1.0000 ± 0.0000	413.7 ± 0.4	413.7 ± 0.4	1.0000 ± 0.0000	1.0000 ± 0.0000	1.00 ± 0.00	2.14 ± 0.10
308.12 ± 0.03	0.4822 ± 0.0052	0.0042 ± 0.0003	0.9914 ± 0.0007	409.4 ± 0.4	410.0 ± 0.6	0.9912 ± 0.0007	0.9991 ± 0.0001	1.00 ± 0.00	2.11 ± 0.09
308.12 ± 0.03	0.4822 ± 0.0052	0.0150 ± 0.0004	0.9698 ± 0.0011	401.0 ± 0.4	401.1 ± 0.7	0.9693 ± 0.0011	0.9969 ± 0.0003	1.00 ± 0.00	2.05 ± 0.08
308.12 ± 0.03	0.4822 ± 0.0052	0.0254 ± 0.0005	0.9499 ± 0.0015	393.3 ± 0.4	393.2 ± 0.8	0.9491 ± 0.0015	0.9950 ± 0.0004	1.00 ± 0.00	1.99 ± 0.06
308.11 ± 0.03	0.4822 ± 0.0052	0.0544 ± 0.0008	0.8986 ± 0.0023	374.1 ± 0.4	373.8 ± 0.8	0.8971 ± 0.0024	0.9902 ± 0.0006	1.01 ± 0.00	1.85 ± 0.04
308.11 ± 0.03	0.4822 ± 0.0052	0.0861 ± 0.0011	0.8485 ± 0.0031	356.6 ± 0.4	356.4 ± 0.6	0.8467 ± 0.0031	0.9858 ± 0.0008	1.02 ± 0.00	1.72 ± 0.02
308.12 ± 0.03	0.4822 ± 0.0052	0.1215 ± 0.0015	0.7987 ± 0.0037	340.3 ± 0.4	340.3 ± 0.6	0.7966 ± 0.0038	0.9817 ± 0.0009	1.03 ± 0.00	1.61 ± 0.01
308.13 ± 0.03	0.4822 ± 0.0052	0.1617 ± 0.0019	0.7489 ± 0.0042	325.1 ± 0.4	325.1 ± 0.6	0.7467 ± 0.0043	0.9778 ± 0.0009	1.05 ± 0.01	1.51 ± 0.01
308.12 ± 0.03	0.4822 ± 0.0052	0.2073 ± 0.0024	0.6993 ± 0.0047	310.1 ± 0.4	310.5 ± 0.5	0.6972 ± 0.0047	0.9740 ± 0.0010	1.08 ± 0.01	1.42 ± 0.00
308.11 ± 0.03	0.4822 ± 0.0052	0.2611 ± 0.0029	0.6487 ± 0.0050	295.5 ± 0.4	296.0 ± 0.5	0.6468 ± 0.0050	0.9700 ± 0.0011	1.11 ± 0.01	1.35 ± 0.00
308.11 ± 0.03	0.4822 ± 0.0052	0.3239 ± 0.0035	0.5982 ± 0.0052	281.4 ± 0.4	281.4 ± 0.5	0.5965 ± 0.0052	0.9659 ± 0.0012	1.14 ± 0.01	1.28 ± 0.00
308.12 ± 0.03	0.4822 ± 0.0052	0.3963 ± 0.0043	0.5489 ± 0.0053	268.3 ± 0.4	266.9 ± 0.5	0.5476 ± 0.0053	0.9616 ± 0.0014	1.18 ± 0.01	1.23 ± 0.00
308.12 ± 0.03	0.4822 ± 0.0052	0.4859 ± 0.0052	0.4981 ± 0.0053	255.4 ± 0.4	251.4 ± 0.6	0.4972 ± 0.0054	0.9566 ± 0.0015	1.22 ± 0.01	1.18 ± 0.00
308.12 ± 0.03	0.4813 ± 0.0052	0.4858 ± 0.0052	0.4977 ± 0.0053	254.2 ± 0.4	251.2 ± 0.6	0.4968 ± 0.0054	0.9566 ± 0.0015	1.22 ± 0.01	1.18 ± 0.00
308.12 ± 0.03	0.3942 ± 0.0043	0.4858 ± 0.0052	0.4480 ± 0.0053	234.8 ± 0.4	234.5 ± 0.7	0.4465 ± 0.0053	0.9509 ± 0.0017	1.27 ± 0.01	1.14 ± 0.00
308.12 ± 0.03	0.3199 ± 0.0035	0.4858 ± 0.0052	0.3971 ± 0.0052	215.7 ± 0.4	216.4 ± 0.8	0.3950 ± 0.0052	0.9439 ± 0.0019	1.32 ± 0.01	1.11 ± 0.00
308.12 ± 0.03	0.2578 ± 0.0029	0.4858 ± 0.0052	0.3467 ± 0.0049	196.5 ± 0.4	197.4 ± 0.9	0.3442 ± 0.0049	0.9354 ± 0.0022	1.37 ± 0.02	1.09 ± 0.00
308.12 ± 0.03	0.2055 ± 0.0023	0.4858 ± 0.0052	0.2973 ± 0.0046	176.9 ± 0.4	177.4 ± 0.9	0.2944 ± 0.0046	0.9249 ± 0.0024	1.43 ± 0.02	1.06 ± 0.00
308.12 ± 0.03	0.1597 ± 0.0019	0.4858 ± 0.0052	0.2475 ± 0.0042	155.8 ± 0.4	156.0 ± 0.7	0.2443 ± 0.0042	0.9108 ± 0.0027	1.50 ± 0.02	1.04 ± 0.00
308.12 ± 0.03	0.1199 ± 0.0014	0.4858 ± 0.0052	0.1979 ± 0.0036	133.2 ± 0.4	133.0 ± 0.6	0.1946 ± 0.0036	0.8911 ± 0.0030	1.58 ± 0.03	1.03 ± 0.00
308.12 ± 0.03	0.0852 ± 0.0011	0.4858 ± 0.0052	0.1492 ± 0.0030	108.9 ± 0.4	108.7 ± 0.4	0.1462 ± 0.0030	0.8617 ± 0.0034	1.68 ± 0.03	1.02 ± 0.00
308.12 ± 0.03	0.0539 ± 0.0008	0.4858 ± 0.0052	0.0999 ± 0.0023	81.8 ± 0.4	81.8 ± 0.5	0.0973 ± 0.0022	0.8095 ± 0.0041	1.79 ± 0.04	1.01 ± 0.00
308.12 ± 0.03	0.0284 ± 0.0005	0.4858 ± 0.0052	0.0553 ± 0.0015	54.8 ± 0.4	54.9 ± 0.5	0.0536 ± 0.0015	0.7071 ± 0.0058	1.92 ± 0.06	1.00 ± 0.00
308.11 ± 0.03	0.0187 ± 0.0004	0.4858 ± 0.0052	0.0371 ± 0.0012	42.8 ± 0.4	43.0 ± 0.6	0.0359 ± 0.0011	0.6213 ± 0.0074	1.98 ± 0.06	1.00 ± 0.00
308.12 ± 0.03	0.0082 ± 0.0003	0.4858 ± 0.0052	0.0167 ± 0.0008	28.9 ± 0.4	28.9 ± 0.7	0.0161 ± 0.0008	0.4284 ± 0.0112	2.06 ± 0.07	1.00 ± 0.00
308.12 ± 0.03	0.0000 ± 0.0000	0.4858 ± 0.0052	0.0000 ± 0.0000	16.7 ± 0.4	16.7 ± 0.4	0.0000 ± 0.0000	0.0000 ± 0.0000	2.13 ± 0.08	1.00 ± 0.00
336.84 ± 0.03	0.4578 ± 0.0049	0.0000 ± 0.0000	1.0000 ± 0.0000	855.5 ± 0.4	855.5 ± 0.4	1.000 ± 0.0000	1.0000 ± 0.0000	1.00 ± 0.00	1.90 ± 0.09
336.84 ± 0.03	0.4578 ± 0.0049	0.0044 ± 0.0003	0.9904 ± 0.0008	846.0 ± 0.4	846.4 ± 0.9	0.9900 ± 0.0008	0.9985 ± 0.0002	1.00 ± 0.00	1.88 ± 0.08
336.84 ± 0.03	0.4578 ± 0.0049	0.0144 ± 0.0004	0.9696 ± 0.0011	827.5 ± 0.4	827.7 ± 1.0	0.9685 ± 0.0012	0.9953 ± 0.0004	1.00 ± 0.00	1.83 ± 0.07
336.85 ± 0.03	0.4578 ± 0.0049	0.0243 ± 0.0005	0.9497 ± 0.0015	809.9 ± 0.4	810.2 ± 1.1	0.9479 ± 0.0016	0.9924 ± 0.0005	1.00 ± 0.00	1.79 ± 0.06
336.85 ± 0.03	0.4578 ± 0.0049	0.0511 ± 0.0008	0.8996 ± 0.0024	768.9 ± 0.4	768.9 ± 1.0	0.8967 ± 0.0025	0.9852 ± 0.0008	1.01 ± 0.00	1.69 ± 0.04
336.85 ± 0.03	0.4578 ± 0.0049	0.0811 ± 0.0011	0.8496 ± 0.0031	730.6 ± 0.4	730.5 ± 0.9	0.8458 ± 0.0032	0.9784 ± 0.0009	1.02 ± 0.00	1.59 ± 0.02
336.85 ± 0.03	0.4578 ± 0.0049	0.1151 ± 0.0014	0.7991 ± 0.0037	694.1 ± 0.4	694.2 ± 0.6	0.7949 ± 0.0039	0.9718 ± 0.0010	1.03 ± 0.00	1.51 ± 0.02
336.84 ± 0.03	0.4578 ± 0.0049	0.1546 ± 0.0018	0.7475 ± 0.0043	658.7 ± 0.4	658.9 ± 0.6	0.7433 ± 0.0044	0.9652 ± 0.0011	1.05 ± 0.01	1.43 ± 0.01
336.84 ± 0.03	0.4578 ± 0.0049	0.1986 ± 0.0023	0.6974 ± 0.0047	625.9 ± 0.4	626.1 ± 0.7	0.6934 ± 0.0048	0.9588 ± 0.0011	1.07 ± 0.01	1.36 ± 0.01
336.84 ± 0.03	0.4578 ± 0.0049	0.2485 ± 0.0028	0.6481 ± 0.0050	594.5 ± 0.4	594.5 ± 0.8	0.6444 ± 0.0051	0.9523 ± 0.0011	1.09 ± 0.01	1.31 ± 0.00
336.85 ± 0.03	0.4578 ± 0.0049	0.3100 ± 0.0034	0.5962 ± 0.0052	562.0 ± 0.4	561.6 ± 0.8	0.5931 ± 0.0053	0.9452 ± 0.0012	1.12 ± 0.01	1.25 ± 0.00
336.85 ± 0.03	0.4578 ± 0.0049	0.3790 ± 0.0041	0.5471 ± 0.0053	531.8 ± 0.4	530.5 ± 0.7	0.5446 ± 0.0054	0.9380 ± 0.0013	1.15 ± 0.01	1.21 ± 0.00
336.85 ± 0.03	0.4578 ± 0.0049	0.4632 ± 0.0049	0.4971 ± 0.0054	501.0 ± 0.4	498.4 ± 0.6	0.4955 ± 0.0054	0.9300 ± 0.0014	1.18 ± 0.01	1.17 ± 0.00
336.84 ± 0.03	0.4609 ± 0.0049	0.4626 ± 0.0049	0.4991 ± 0.0054	500.6 ± 0.4	499.5 ± 0.6	0.4975 ± 0.0054	0.9303 ± 0.0013	1.18 ± 0.01	1.17 ± 0.00
336.84 ± 0.03	0.3783 ± 0.0041	0.4626 ± 0.0049	0.4499 ± 0.0053	465.5 ± 0.4	465.5 ± 0.4	0.4472 ± 0.0054	0.9211 ± 0.0015	1.22 ± 0.01	1.14 ± 0.00
336.84 ± 0.03	0.3078 ± 0.0034	0.4626 ± 0.0049	0.3995 ± 0.0052	428.9 ± 0.4	429.5 ± 0.5	0.3958 ± 0.0052	0.9101 ± 0.0016	1.27 ± 0.02	1.11 ± 0.00
336.84 ± 0.03	0.2499 ± 0.0028	0.4626 ± 0.0049	0.3507 ± 0.0050	392.5 ± 0.4	393.0 ± 0.6	0.3461 ± 0.0050	0.8974 ± 0.0017	1.32 ± 0.02	1.08 ± 0.00
336.83 ± 0.03	0.1975 ± 0.0022	0.4626 ± 0.0049	0.2991 ± 0.0046	352.2 ± 0.4	352.5 ± 0.6	0.2938 ± 0.0046	0.8805 ± 0.0018	1.38 ± 0.02	1.06 ± 0.00
336.84 ± 0.03	0.1521 ± 0.0018	0.4626 ± 0.0049	0.2474 ± 0.0042	309.3 ± 0.4	309.3 ± 0.6	0.2416 ± 0.0042	0.8584 ± 0.0019	1.45 ± 0.02	1.04 ± 0.00
336.84 ± 0.03	0.1138 ± 0.0014	0.4626 ± 0.0049	0.1974 ± 0.0036	264.9 ± 0.4	264.8 ± 0.6	0.1915 ± 0.0036	0.8285 ± 0.0020	1.52 ± 0.03	1.03 ± 0.00
336.84 ± 0.03	0.0802 ± 0.0010	0.4626 ± 0.0049	0.1477 ± 0.003	217.5 ± 0.4	217.4 ± 0.7	0.1422 ± 0.0029	0.7841 ± 0.0020	1.61 ± 0.03	1.01 ± 0.00
336.84 ± 0.03	0.0505 ± 0.0007	0.4626 ± 0.0049	0.0984 ± 0.0023	166.7 ± 0.4	166.7 ± 0.7	0.0940 ± 0.0022	0.7096 ± 0.0021	1.71 ± 0.04	1.01 ± 0.00
336.84 ± 0.03	0.0241 ± 0.0005	0.4626 ± 0.0049	0.0495 ± 0.0014	111.8 ± 0.4	111.9 ± 0.5	0.0468 ± 0.0014	0.5547 ± 0.0026	1.82 ± 0.05	1.00 ± 0.00
336.84 ± 0.03	0.0143 ± 0.0004	0.4626 ± 0.0049	0.0301 ± 0.0011	88.7 ± 0.4	88.8 ± 0.6	0.0283 ± 0.0010	0.4326 ± 0.0037	1.87 ± 0.06	1.00 ± 0.00
336.84 ± 0.03	0.0029 ± 0.0002	0.4626 ± 0.0049	0.0062 ± 0.0006	59.2 ± 0.4	59.1 ± 0.9	0.0058 ± 0.0006	0.1371 ± 0.0087	1.93 ± 0.07	1.00 ± 0.00
336.83 ± 0.03	0.0000 ± 0.0000	0.4626 ± 0.0049	0.0000 ± 0.0000	51.2 ± 0.4	51.2 ± 0.4	0.0000 ± 0.0000	0.0000 ± 0.0000	1.95 ± 0.07	1.00 ± 0.00

[a] Experimental temperature T; amount of component in the equilibrium cell n_i; total mole fraction z_1; experimental pressure p_{measd}; pressure calculated from the Legendre polynomial fit p_{Leg}; liquid and vapor phase equilibrium mole fractions x_1 and y_1; activity coefficients γ_1 and γ_2.

dx.doi.org/10.1021/je101343m |J. Chem. Eng. Data 2011, 56, 614–621

Table 9. VLE Data for *trans*-But-2-ene (1) + Thiophene (2)[a]

T/K	n_1/mol	n_2/mol	z_1	p_{measd}/kPa	p_{Leg}/kPa	x_1	y_1	γ_1	γ_2
308.14 ± 0.03	0.4948 ± 0.0053	0.0000 ± 0.0000	1.0000 ± 0.0000	317.3 ± 0.4	317.3 ± 0.4	1.0000 ± 0.0000	1.0000 ± 0.0000	1.00 ± 0.00	2.00 ± 0.09
308.15 ± 0.03	0.4948 ± 0.0053	0.0056 ± 0.0003	0.9888 ± 0.0007	313.8 ± 0.4	313.8 ± 0.6	0.9887 ± 0.0008	0.9987 ± 0.0002	1.00 ± 0.00	1.97 ± 0.08
308.15 ± 0.03	0.4948 ± 0.0053	0.0149 ± 0.0004	0.9708 ± 0.0011	308.4 ± 0.4	308.4 ± 0.6	0.9705 ± 0.0011	0.9966 ± 0.0003	1.00 ± 0.00	1.92 ± 0.07
308.15 ± 0.03	0.4948 ± 0.0053	0.0255 ± 0.0005	0.9509 ± 0.0014	302.5 ± 0.4	302.5 ± 0.7	0.9503 ± 0.0015	0.9943 ± 0.0005	1.00 ± 0.00	1.87 ± 0.06
308.15 ± 0.03	0.4948 ± 0.0053	0.0563 ± 0.0008	0.8979 ± 0.0023	287.6 ± 0.4	287.6 ± 0.7	0.8968 ± 0.0024	0.9885 ± 0.0008	1.01 ± 0.00	1.75 ± 0.04
308.15 ± 0.03	0.4948 ± 0.0053	0.0881 ± 0.0011	0.8489 ± 0.0031	274.6 ± 0.4	274.7 ± 0.7	0.8476 ± 0.0031	0.9833 ± 0.0010	1.02 ± 0.00	1.65 ± 0.03
308.14 ± 0.03	0.4948 ± 0.0053	0.1252 ± 0.0015	0.7981 ± 0.0037	261.8 ± 0.4	261.9 ± 0.6	0.7966 ± 0.0038	0.9781 ± 0.0011	1.03 ± 0.00	1.55 ± 0.02
308.14 ± 0.03	0.4948 ± 0.0053	0.1666 ± 0.0019	0.7481 ± 0.0042	249.7 ± 0.4	249.8 ± 0.6	0.7466 ± 0.0043	0.9730 ± 0.0012	1.05 ± 0.01	1.47 ± 0.01
308.14 ± 0.03	0.4948 ± 0.0053	0.2135 ± 0.0024	0.6986 ± 0.0047	238.1 ± 0.4	238.2 ± 0.6	0.6971 ± 0.0047	0.9679 ± 0.0014	1.07 ± 0.01	1.40 ± 0.01
308.14 ± 0.03	0.4948 ± 0.0053	0.2677 ± 0.0030	0.6489 ± 0.005	226.7 ± 0.4	226.7 ± 0.6	0.6475 ± 0.0050	0.9627 ± 0.0015	1.09 ± 0.01	1.34 ± 0.00
308.14 ± 0.03	0.4948 ± 0.0053	0.3295 ± 0.0036	0.6003 ± 0.0052	215.7 ± 0.4	215.6 ± 0.5	0.5991 ± 0.0052	0.9573 ± 0.0016	1.12 ± 0.01	1.29 ± 0.00
308.14 ± 0.03	0.4948 ± 0.0053	0.4040 ± 0.0043	0.5505 ± 0.0053	204.4 ± 0.4	204.2 ± 0.5	0.5496 ± 0.0053	0.9515 ± 0.0017	1.15 ± 0.01	1.24 ± 0.00
308.14 ± 0.03	0.4948 ± 0.0053	0.4931 ± 0.0052	0.5008 ± 0.0053	192.9 ± 0.4	192.6 ± 0.5	0.5003 ± 0.0053	0.9452 ± 0.0019	1.19 ± 0.01	1.19 ± 0.00
308.14 ± 0.03	0.4948 ± 0.0053	0.4957 ± 0.0053	0.4995 ± 0.0053	192.3 ± 0.4	192.3 ± 0.5	0.4989 ± 0.0053	0.9450 ± 0.0019	1.19 ± 0.01	1.19 ± 0.00
308.14 ± 0.03	0.4058 ± 0.0044	0.4957 ± 0.0053	0.4501 ± 0.0053	180.2 ± 0.4	180.2 ± 0.5	0.4491 ± 0.0053	0.9379 ± 0.0021	1.23 ± 0.01	1.16 ± 0.00
308.14 ± 0.03	0.3305 ± 0.0036	0.4957 ± 0.0053	0.4000 ± 0.0052	167.4 ± 0.4	167.4 ± 0.5	0.3986 ± 0.0052	0.9295 ± 0.0023	1.28 ± 0.02	1.12 ± 0.00
308.13 ± 0.03	0.2669 ± 0.0030	0.4957 ± 0.0053	0.3500 ± 0.0050	154.0 ± 0.4	154.0 ± 0.5	0.3482 ± 0.0050	0.9195 ± 0.0025	1.34 ± 0.02	1.09 ± 0.00
308.14 ± 0.03	0.2136 ± 0.0024	0.4957 ± 0.0053	0.3012 ± 0.0046	139.9 ± 0.4	139.9 ± 0.5	0.2991 ± 0.0046	0.9074 ± 0.0027	1.40 ± 0.02	1.07 ± 0.00
308.14 ± 0.03	0.1668 ± 0.0019	0.4957 ± 0.0053	0.2518 ± 0.0042	124.6 ± 0.4	124.6 ± 0.4	0.2495 ± 0.0042	0.8915 ± 0.003	1.48 ± 0.02	1.05 ± 0.00
308.14 ± 0.03	0.1240 ± 0.0015	0.4957 ± 0.0053	0.2001 ± 0.0036	107.0 ± 0.4	107.0 ± 0.5	0.1977 ± 0.0036	0.8681 ± 0.0034	1.57 ± 0.03	1.03 ± 0.00
308.13 ± 0.03	0.0881 ± 0.0011	0.4957 ± 0.0053	0.1509 ± 0.0030	88.4 ± 0.4	88.4 ± 0.5	0.1486 ± 0.0030	0.8339 ± 0.0039	1.66 ± 0.04	1.02 ± 0.00
308.14 ± 0.03	0.0561 ± 0.0008	0.4957 ± 0.0053	0.1016 ± 0.0023	67.7 ± 0.4	67.7 ± 0.5	0.0997 ± 0.0023	0.7746 ± 0.0046	1.78 ± 0.04	1.01 ± 0.00
308.14 ± 0.03	0.0269 ± 0.0005	0.4957 ± 0.0053	0.0515 ± 0.0014	44.1 ± 0.4	44.1 ± 0.4	0.0503 ± 0.0014	0.6398 ± 0.0062	1.90 ± 0.06	1.00 ± 0.00
308.14 ± 0.03	0.0159 ± 0.0004	0.4957 ± 0.0053	0.0311 ± 0.0011	33.6 ± 0.4	33.6 ± 0.5	0.0303 ± 0.0010	0.5198 ± 0.0077	1.96 ± 0.06	1.00 ± 0.00
308.14 ± 0.03	0.0053 ± 0.0003	0.4957 ± 0.0053	0.0106 ± 0.0007	22.5 ± 0.4	22.5 ± 0.6	0.0104 ± 0.0006	0.2725 ± 0.0113	2.02 ± 0.07	1.00 ± 0.00
308.13 ± 0.03	0.0000 ± 0.0000	0.4957 ± 0.0053	0.0000 ± 0.0000	16.5 ± 0.4	16.5 ± 0.4	0.0000 ± 0.0000	0.0000 ± 0.0000	2.05 ± 0.07	1.00 ± 0.00
335.86 ± 0.03	0.4702 ± 0.0050	0.0000 ± 0.0000	1.0000 ± 0.0000	666.1 ± 0.4	666.1 ± 0.4	1.0000 ± 0.0000	1.0000 ± 0.0000	1.00 ± 0.00	1.83 ± 0.08
335.86 ± 0.03	0.4702 ± 0.0050	0.0039 ± 0.0003	0.9917 ± 0.0007	660.2 ± 0.4	660.5 ± 0.8	0.9915 ± 0.0007	0.9986 ± 0.0002	1.00 ± 0.00	1.82 ± 0.07
335.86 ± 0.03	0.4702 ± 0.0050	0.0147 ± 0.0004	0.9696 ± 0.0011	645.8 ± 0.4	646.0 ± 0.9	0.9688 ± 0.0012	0.9948 ± 0.0004	1.00 ± 0.00	1.77 ± 0.06
335.87 ± 0.03	0.4702 ± 0.0050	0.0250 ± 0.0005	0.9494 ± 0.0015	632.9 ± 0.4	633.2 ± 0.9	0.9482 ± 0.0016	0.9914 ± 0.0006	1.00 ± 0.00	1.73 ± 0.05
335.86 ± 0.03	0.4702 ± 0.0050	0.0534 ± 0.0008	0.8981 ± 0.0024	601.6 ± 0.4	602.0 ± 1.0	0.8959 ± 0.0024	0.9831 ± 0.0009	1.01 ± 0.00	1.63 ± 0.04
335.86 ± 0.03	0.4702 ± 0.0050	0.0852 ± 0.0011	0.8467 ± 0.0031	572.0 ± 0.4	572.5 ± 0.9	0.8440 ± 0.0032	0.9751 ± 0.0011	1.01 ± 0.00	1.55 ± 0.02
335.86 ± 0.03	0.4702 ± 0.0050	0.1200 ± 0.0015	0.7967 ± 0.0037	544.8 ± 0.4	545.3 ± 0.8	0.7937 ± 0.0038	0.9674 ± 0.0012	1.03 ± 0.00	1.47 ± 0.02
335.87 ± 0.03	0.4702 ± 0.0050	0.1577 ± 0.0019	0.7488 ± 0.0042	519.8 ± 0.4	520.2 ± 0.7	0.7458 ± 0.0043	0.9601 ± 0.0013	1.04 ± 0.00	1.41 ± 0.01
335.87 ± 0.03	0.4702 ± 0.0050	0.2027 ± 0.0023	0.6988 ± 0.0047	494.5 ± 0.4	494.8 ± 0.7	0.6958 ± 0.0048	0.9524 ± 0.0014	1.06 ± 0.01	1.35 ± 0.01
335.86 ± 0.03	0.4702 ± 0.0050	0.2545 ± 0.0028	0.6489 ± 0.0050	469.8 ± 0.4	470.0 ± 0.6	0.6462 ± 0.0051	0.9444 ± 0.0014	1.08 ± 0.01	1.30 ± 0.01
335.87 ± 0.03	0.4702 ± 0.0050	0.3147 ± 0.0034	0.5991 ± 0.0052	445.5 ± 0.4	445.5 ± 0.6	0.5968 ± 0.0053	0.9362 ± 0.0015	1.10 ± 0.01	1.25 ± 0.00
335.87 ± 0.03	0.4702 ± 0.0050	0.3861 ± 0.0042	0.5491 ± 0.0053	421.1 ± 0.4	420.9 ± 0.6	0.5474 ± 0.0054	0.9273 ± 0.0015	1.13 ± 0.01	1.21 ± 0.00
335.87 ± 0.03	0.4702 ± 0.0050	0.4698 ± 0.0050	0.5002 ± 0.0053	397.2 ± 0.4	396.7 ± 0.6	0.4991 ± 0.0054	0.9179 ± 0.0016	1.16 ± 0.01	1.17 ± 0.00
335.87 ± 0.03	0.4719 ± 0.0051	0.4743 ± 0.0051	0.4987 ± 0.0053	396.0 ± 0.4	395.9 ± 0.6	0.4976 ± 0.0054	0.9176 ± 0.0016	1.17 ± 0.01	1.17 ± 0.00
335.87 ± 0.03	0.3870 ± 0.0042	0.4743 ± 0.0051	0.4493 ± 0.0053	370.1 ± 0.4	370.1 ± 0.5	0.4474 ± 0.0053	0.9067 ± 0.0017	1.20 ± 0.01	1.14 ± 0.00
335.87 ± 0.03	0.3163 ± 0.0035	0.4743 ± 0.0051	0.4001 ± 0.0052	343.5 ± 0.4	343.5 ± 0.5	0.3974 ± 0.0052	0.8941 ± 0.0018	1.25 ± 0.02	1.11 ± 0.00
335.87 ± 0.03	0.2556 ± 0.0028	0.4743 ± 0.0051	0.3502 ± 0.0050	315.4 ± 0.4	315.4 ± 0.5	0.3468 ± 0.0050	0.8790 ± 0.0019	1.30 ± 0.02	1.08 ± 0.00
335.87 ± 0.03	0.2043 ± 0.0023	0.4743 ± 0.0051	0.3010 ± 0.0046	286.1 ± 0.4	286.1 ± 0.5	0.2971 ± 0.0046	0.8607 ± 0.0020	1.36 ± 0.02	1.06 ± 0.00
335.87 ± 0.03	0.1597 ± 0.0019	0.4743 ± 0.0051	0.2519 ± 0.0042	255.1 ± 0.4	255.0 ± 0.5	0.2476 ± 0.0042	0.8373 ± 0.0022	1.42 ± 0.02	1.04 ± 0.00
335.87 ± 0.03	0.1193 ± 0.0014	0.4743 ± 0.0051	0.2010 ± 0.0037	220.3 ± 0.4	220.4 ± 0.5	0.1966 ± 0.0036	0.8041 ± 0.0022	1.50 ± 0.03	1.03 ± 0.00
335.87 ± 0.03	0.0845 ± 0.0011	0.4743 ± 0.0051	0.1512 ± 0.0030	183.6 ± 0.4	183.6 ± 0.6	0.1470 ± 0.0030	0.7561 ± 0.0023	1.58 ± 0.03	1.01 ± 0.00
335.87 ± 0.03	0.0536 ± 0.0008	0.4743 ± 0.0051	0.1015 ± 0.0023	143.6 ± 0.4	143.7 ± 0.6	0.0981 ± 0.0023	0.6770 ± 0.0023	1.67 ± 0.04	1.01 ± 0.00
335.87 ± 0.03	0.0257 ± 0.0005	0.4743 ± 0.0051	0.0514 ± 0.0014	99.5 ± 0.4	99.5 ± 0.6	0.0493 ± 0.0014	0.5177 ± 0.0030	1.78 ± 0.05	1.00 ± 0.00
335.88 ± 0.03	0.0158 ± 0.0004	0.4743 ± 0.0051	0.0322 ± 0.0011	81.5 ± 0.4	81.5 ± 0.7	0.0308 ± 0.0011	0.4034 ± 0.0041	1.83 ± 0.05	1.00 ± 0.00
335.88 ± 0.03	0.0059 ± 0.0003	0.4743 ± 0.0051	0.0122 ± 0.0007	62.0 ± 0.4	61.9 ± 0.8	0.0117 ± 0.0007	0.2054 ± 0.0066	1.87 ± 0.06	1.00 ± 0.00
335.87 ± 0.03	0.0000 ± 0.0000	0.4743 ± 0.0051	0.0000 ± 0.0000	49.6 ± 0.4	49.6 ± 0.4	0.0000 ± 0.0000	0.0000 ± 0.0000	1.91 ± 0.06	1.00 ± 0.00

[a] Experimental temperature T; amount of component in the equilibrium cell n_i; total mole fraction z_1; experimental pressure p_{measd}; pressure calculated from the Legendre polynomial fit p_{Leg}; liquid and vapor phase equilibrium mole fractions x_1 and y_1; activity coefficients γ_1 and γ_2.

dx.doi.org/10.1021/je101343m |J. Chem. Eng. Data 2011, 56, 614–621

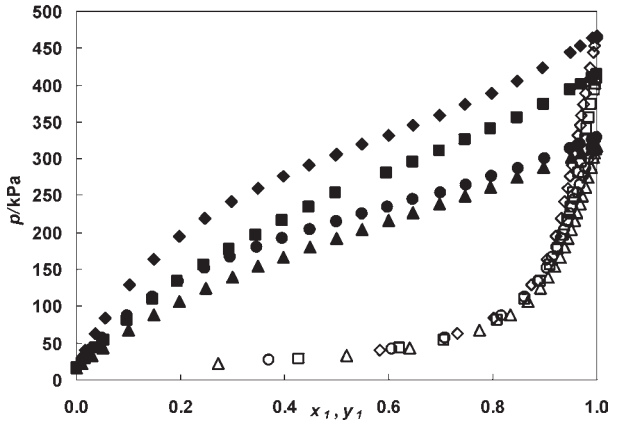

Figure 1. Experimental pressure, p, and liquid and vapor phase equilibrium composition, x_1 and y_1, in mole fractions at 308 K of thiophene (2) + butane, ●, x and ○, y; + 2-methylpropane, ♦, x and ◊, y; + 2-methylpropene, ■, x and □, y; + *trans*-but-2-ene, ▲, x and △, y, measured at 308 K.

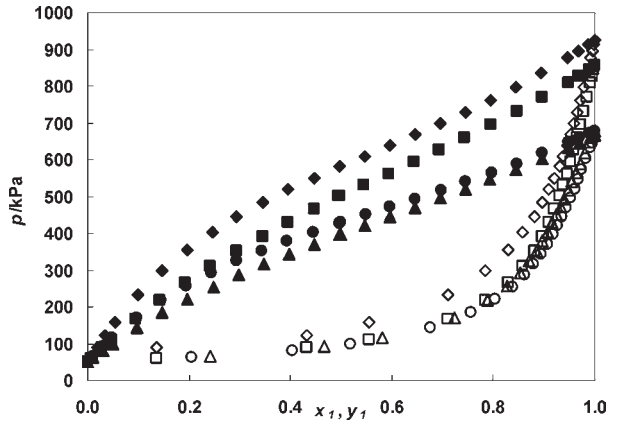

Figure 2. Experimental pressure, p and liquid and vapor phase equilibrium composition (x_1 and y_1) in mole fractions at 336 K of thiophene (2) + butane, ●, x and ○, y; + 2-methylpropane, ♦, x and ◊, y; + 2-methylpropene, ■, x and □, y; + *trans*-but-2-ene, ▲, x and △, y, measured at 308 K.

reduced by the Legendre polynomials as the liquid activity coefficient model.[7] The cubic Soave−Redlich−Kwong (SRK)[8] equation of state was used as the fugacity coefficient model for the vapor phase. The binary interaction parameters of SRK equation of state for the systems were set to 0. The data reduction was performed according to the Barker method.[9] The amount of parameters for Legendre polynomials[7] was increased until the absolute average deviation was below the uncertainty in the measured cell pressure. The details of this data reduction have been reported by Uusi-Kyyny et al.[6] The data were reduced with our in-house software, VLEFIT.[10] Compound properties used in the data reduction are shown in Table 3. The data reduction was also made with the Wilson model.[11]

Error Analysis. The values of the experimental uncertainties are presented in Table 4. Uncertainties connected to the addition of components to the equilibrium cell are as follows: the maximum uncertainty in the liquid density correlation was estimated as the maximum absolute average error between the data sets used to obtain the correlation and the corresponding

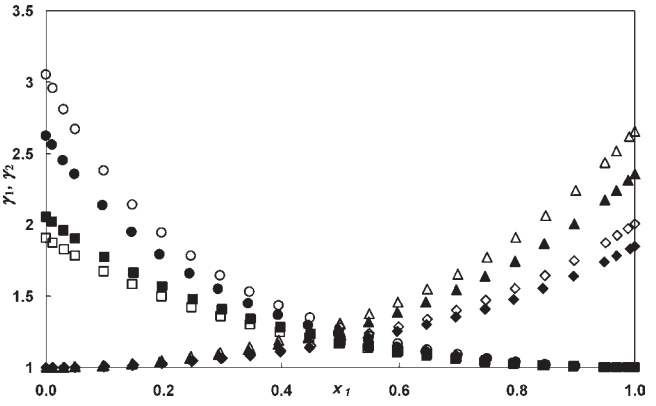

Figure 3. Activity coefficients γ_1 and γ_2 at liquid phase mole fraction x_1. ○, Butane (1) + △, thiophene system at 308 K; ●, butane (1) + ▲, thiophene system at 336 K; ■, trans-but-2-ene (1) + ◊, thiophene system at 308 K; □, *trans*-but-2-ene (1) + ♦, thiophene system at 336 K.

calculated value at temperatures from (270 to 310) K. The temperature range was determined by the pump operating temperature which was kept at approximately 288 K. Calibration experiments with distilled water were used to determine the uncertainty in the injection volume. Also, the pump temperature and pressure were recorded and used for an accurate as possible description of the liquid density taking into account isothermal compressibility.

Uncertainties of the equilibrium cell measurements are as follows: the uncertainty in the reduced data depended on the uncertainty in the measured values of the temperature, the pressure, and the overall molar composition. The maximum theoretical error of the overall molar composition was calculated by the method presented by Hynynen et al.[12] Maximum uncertainty of the reduced data was obtained by alternating the measurement uncertainties between their minimum and maximum values, one at a time, and calculating the average deviation of the results.[13,14]

■ RESULTS AND DISCUSSION

The measured pure component vapor pressures agreed well with the pressures calculated with literature correlations, as shown in Table 2. The total pressure of each measured system coincided well at the equimolar composition. The experimental data were regressed separately for each data set to obtain gas and liquid phase mole fractions. Legendre polynomials[7] were used as the liquid activity coefficient model and the cubic SRK equation of state for the vapor phase fugacity coefficients.[8] The number of parameters for the Legendre polynomials was increased until the pressure absolute average deviation was below the uncertainty of the cell pressure measurement. This could be achieved in all of the data sets except for the 2-methylpropene + thiophene system at 308 K. The activity coefficient model parameters with absolute average pressure residuals and activity coefficients at infinite dilution are presented in Table 5. No more than four parameters were needed in any of the regressed sets. Increasing the amount of parameters did not provide any substantial improvement in the absolute average pressure residual.

The measured data, regressed equilibrium phase compositions, and activity coefficients are shown in Tables 6 to 9. Equilibrium phase compositions are presented in Figures 1 and 2. All measured binary systems showed a positive deviation from

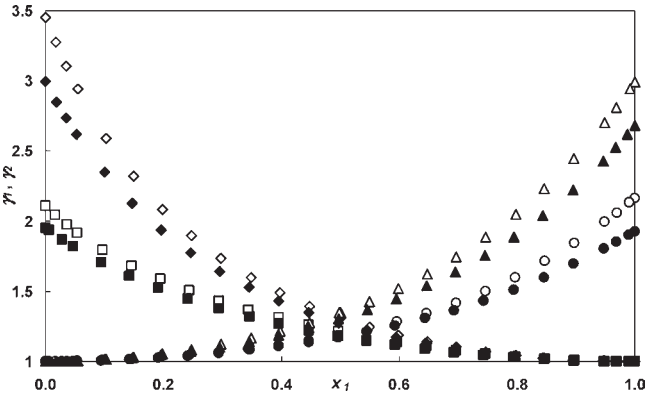

Figure 4. Activity coefficients γ_1 and γ_2 at liquid phase mole fraction x_1. ◇, 2-Methylpropane (1) + △, thiophene system at 308 K; ◆, 2-methylpropane (1) + ▲, thiophene system at 336 K; □, 2-methylpropene (1) + ○, thiophene system at 308 K; ■, 2-methylpropene (1) + ●, thiophene system at 336 K.

Raoult's law. The systems showed weak temperature dependency, as shown in the liquid activity coefficient graphs in Figures 3 and 4. The data were considered to be of good quality.

Additionally, the Wilson equation was used for the regression of the measurements with the Barker method. The infinite dilution activity coefficient values obtained with the Wilson model were close to the ones obtained from the regression using the Legendre polynomials. Also, the average absolute pressure residuals were typical according to our experiences. This means that the Wilson model could describe each system, adequately at both measured temperatures, with only two parameters.

AUTHOR INFORMATION

Corresponding Author

*Fax: +358 9 470 22694. E-mail: petri.uusi-kyyny@tkk.fi.

REFERENCES

(1) Vistisen, P.-Ø.; Zeuthen, P. Reactions of organic sulfur and nitrogen compounds in the FCC pretreater and the FCC unit. *Ind. Eng. Chem. Res.* **2008**, *47*, 8471–8477.

(2) Krause, O. I. A.; Keskinen, K. Etherification. In *Handbook of heterogeneous catalysis*, 2nd ed., Vol. 6; Ertl, G., Knözinger, H., Schüth, F., Weitkamp, J., Eds.; Wiley: New York, 2008; pp 2864−2881

(3) Van Ness, H. C.; Abbott, M. A procedure for rapid degassing of liquids. *Ind. Eng. Chem. Fundam.* **1978**, *17*, 66–67.

(4) Fischer, K.; Gmehling, J. P-x and $\gamma\infty$ data for the different binary butanol-water systems at 50 °C. *J. Chem. Eng. Data* **1994**, *39*, 309–315.

(5) Fawcett, F. S.; Rasmussen, H. E. Physical properties of thiophene. *J. Am. Chem. Soc.* **1945**, *67*, 1705–1709.

(6) Uusi-Kyyny, P.; Pokki, J.-P.; Laakkonen, M.; Aittamaa, J.; Liukkonen, S. Vapor liquid equilibrium for the binary systems 2-methylpentane + 2-butanol at 329.2 K and n-hexane + 2-butanol at 329.2 and 373.2 K with a static apparatus. *Fluid Phase Equilib.* **2002**, *201*, 343–358.

(7) Gmehling, J.; Onken, U. *Vapour-Liquid Data Collection; DECHEMA Chemistry Data Series, Part 1*; DECHEMA: Frankfurt/Main, 1977; Vol. 1.

(8) Soave, G. Equilibrium constants from a modified Redlich-Kwong equation of state. *Chem. Eng. Sci.* **1972**, *27*, 1197–1203.

(9) Barker, J. A. Determination of activity coefficients from total pressure measurements. *Aust. J. Chem.* **1953**, *6*, 207–210.

(10) Aittamaa, J.; Pokki, J.-P. *User Manual of Program VLEFIT*; Helsinki University of Technology: Espoo, Finland, 2003. http://chemtech.tkk.fi/en/research/chemical_engineering/software/web_-flowbat_ja_web_vlefit/.

(11) Wilson, G. M. Vapor-Liquid Equilibrium. XI. A new expression for the excess free energy of mixing. *J. Am. Chem. Soc.* **1964**, *86*, 127–130.

(12) Hynynen, K.; Uusi-Kyyny, P.; Pokki, J.-P.; Pakkanen, M.; Aittamaa, J. Isothermal Vapor Liquid Equilibrium for 2-Methylpropene + Methanol, + 1-Propanol, + 2-Propanol, + 2-Butanol, and + 2-Methyl-2-propanol Binary Systems at 364.5 K. *J. Chem. Eng. Data* **2006**, *51*, 562–568.

(13) Laakkonen, M.; Pokki, J.-P.; Uusi-Kyyny, P.; Aittamaa, J. Vapor-liquid equilibrium for the 1-butene + methanol, + ethanol, + 2-propanol, + 2-butanol and + 2-methyl-2-propanol systems at 326 K. *Fluid Phase Equilib.* **2003**, *212*, 237–252.

(14) Sundberg, A.; Uusi-Kyyny, P.; Pakkanen, M.; Pokki, J.-P.; Alopaeus, V. Vapor-Liquid Equilibrium for Tetrahydrothiophene + n-Butane, + trans-2-Butene, + 2-Methylpropane, and + 2-Methylpropene. *J. Chem. Eng. Data* **2009**, *54*, 1311–1317.

(15) Reid, R. C.; Prausnitz, J. M.; Poling, B. E. *The properties of gases and liquids*, 4th ed.; McGraw-Hill: New York, 1988.

(16) Yaws, C. L. *Yaws' Handbook of Thermodynamic and Physical Properties of Chemical Compounds*; Gulf Publishing Company: Houston, TX, 2003; accessed at http://www.knovel.com.

(17) Design Institute for Physical Properties. *DIPPR Project 801 - Full Version*; Design Institute for Physical Property Research/AIChE, 2005; 2008; 2009; 2010; accessed at http://www.knovel.com.