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Vapor−Liquid Equilibrium for Dimethyl Disulfide + Butane, + *trans*-But-2-ene, + 2-Methylpropane, + 2-Methylpropene, + Ethanol, and 2-Ethoxy-2-methylpropane

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ABSTRACT: Isothermal vapor−liquid equilibrium (VLE) of binary systems of dimethyl disulfide (DMDS) + butane, + *trans*-but-2-ene, + 2-methylpropane, and + 2-methylpropene was measured at 350 K with a static total pressure apparatus. The measured data were reduced to phase equilibrium data with the Barker's method. Additionally, a circulation still was used to measure isothermal VLE of binary systems of DMDS + ethanol and + 2-ethoxy-2-methylpropane (ETBE) at 343.15 K. The DMDS + ethanol system showed azeotropic behavior. All binary systems measured exhibited a positive deviation from Raoult's Law.

INTRODUCTION

Sulfur content in liquid fuels is stringently regulated by legislation to reduce air pollution. One of the components contributing to the sulfur content in liquid fuels is dimethyl disulfide.[1] It is important to know the phase behavior of organic sulfur components to be able to control the sulfur content of process streams.[2] Process streams originating from the Fluid Catalytic Cracker (FCC) unit contribute to a large extent to the amount 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 the octane number of the fuel, and is one method to introduce bioethanol to the gasoline pool.[3] 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 distributions 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 determination of the ether product stream.

The target of this work was to measure VLE data for DMDS with C4 hydrocarbons, ethanol, and ETBE. The measurements were made for the systems DMDS + butane, + *trans*-but-2-ene, + 2-methylpropane, and + 2-methylpropene at 350 K. The measurements of the DMDS + ethanol, and + ETBE were made at 343.15 K.

EXPERIMENTAL SECTION

Materials. The suppliers and the purities of the materials used are presented in Table 1. DMDS, ethanol, and ETBE were analyzed with a GC, equipped with a flame ionization detector, which does not detect the presence of water. The ETBE was further purified by distillation and extraction of alcohol impurities with distilled water. The DMDS, ethanol, and ETBE were dried over molecular sieves (Merck, 3A), and the water content was analyzed with Karl Fischer titration. Success of the purification was determined, in addition to the GC analysis, by comparing the measured vapor pressure and the refractive index with values obtained from the literature, as presented in Tables 1 and 2. The refractive indexes, n_D, of the pure liquids were measured at 298.15 K with ABBEMAT-HP automatic refractometer (Dr. Kernchen, Germany) with accuracy ±0.00002. The measured refractive indexes corresponded well with literature values.[4,5]

The degassing of DMDS for the static total pressure measurements was performed by vacuum suction of DMDS placed in a round-bottom flask. The round-bottom flask was placed in an ultra sonic bath. Water ice was added to the water container of the ultra sonic bath for reducing the amount of DMDS drawn to the trap cooled with liquid nitrogen. The degassing setup is presented in Figure 1.

Vapor pressures are shown in Table 2. Each reported pure component vapor pressure value was separately measured in separate VLE runs. The volatile components; C4 alkanes and C4 alkenes were degassed in the syringe pump before use by opening the vacuum valve 10 times for a period of 10 s.

Apparatus. The static total pressure apparatus employed in the experiment has been explained 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).

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Table 1. Supplier and the Purity of the Compounds

			n_D(298 K)	
compound	company	purity mass fraction	measd	lit.
butane	Messer Finland Oy	0. 998	na	na
2-methylpropane	Riedel-de Haën	0.998	na	na
2-methylpropene	Riedel-de Haën	0.998	na	na
trans-but-2-ene	Fluka	>0.998	na	na
DMDS	Sigma-Aldrich	0.998	1.5226	1.523[a]
ethanol	Altia	0.9993	1.3593	1.3594[a]
ETBE	Neste Oil	0.9997	1.3730	1.3729[a]
o-xylene (used as diluent)	Sigma-Aldrich	0.9943	1.5026	1.5029[a]

[a] Reference 4.

Table 2. Pure Compound Vapor Pressure, P, at Temperature T[a]

compound	T/K	P/kPa	P/kPa[b]	P/kPa[c]	P/kPa[d]
butane	308.15	328.8	329.0	328.9	329.2
2-methylpropane	308.14	467.4	468.1	465.8	461.9
2-methylpropene	308.13	413.7	411.3	407	404.6
trans-but-2-ene	308.14	317.3	317.3	317.3	na
DMDS	308.14	17.1	16.6	16.6	16.7
	335.84	49.6	49.8	49.7	49.8
	308.15	17.1	16.7	16.6	16.7
	335.61	49.7	49.4	49.3	49.4
	343.15	27.8	27.7	27.7	na
	343.15	27.8	27.7	27.7	na
ethanol	343.15	72.5	71.9	72.4	72.5
ETBE	343.15	92.9	na	93.8	na

[a] na = not available in references in *b*, *c*, and *d*. [b] Reference 4. [c] Reference 4. [d] Reference 23.

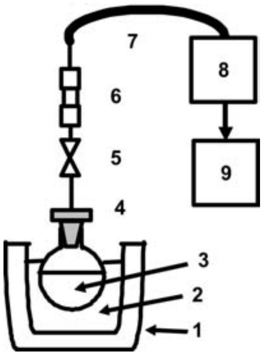

Figure 1. Ultrasonic degassing setup: 1, ultrasonic bath; 2, water with ice; 3, component in degassing; 4, stainless steel adapter fitted to a glass-ground joint; 5, 1/8 in. ball valve; 6, Ultra Torr union connected to 1/8 in. tubing; 7, vacuum hose; 8, trap cooled with liquid nitrogen; 9, vacuum pump.

The circulation still used in the measurements was of the Yerazunis-type[7] with minor modifications to the original design.[8] The experimental setup is described in detail in the previous works.[8,9] Approximately 80 mL of reagents was needed to run the apparatus. Temperatures were measured with a Pt-100 resistance temperature probe, which was located at the bottom of the packed section of the equilibrium chamber and connected to a thermometer (F200, Tempcontrol) with a manufacturer's stated accuracy of ±0.02 K and the calibration uncertainty was ±0.01 K. The uncertainty of the whole temperature measurement system is estimated to be ±0.05 K.

Pressure was measured with a Druck pressure transducer PMP 4070 (0 to 100 kPa) connected to a Red Lion panel meter. The inaccuracy of the instruments was reported to be ±0.07 kPa by the manufacturer. The pressure measurement system was calibrated against a BEAMEX PC 105−1166 pressure calibrator. The uncertainty of the whole pressure measurement system including the calibration uncertainty is expected to be less than ±0.17 kPa.

Procedure. *Static Total Pressure Measurements.* 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 correlation. If the error was within an acceptable limit, the second compound was added into the cell, and after the pressure had reached equilibrium, in about 30 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 the DMDS containing C4 components was directed to the ventilation through a cold trap and an adsorber tube filled with active carbon. The rest of the material in the cell (mostly DMDS) was removed by drawing a reduced pressure to the cell with a vacuum pump. The DMDS was captured in a cold trap cooled with liquid nitrogen.

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 on the basis of how well the vapor pressure of each half coincided at the equimolar composition and how well the measured pure component vapor pressure agreed with the values reported in the literature.

Recirculation Still Measurements. Pure component 1 was introduced in the recirculation still and its vapor pressure was measured at several temperatures. Then component 2 was introduced into the recirculation still. It took approximately (45 to 60) min to achieve constant temperature. The temperature was held constant for approximately (30 to 45) min before sampling. Steady temperature was assumed as indication that phase equilibrium was reached.

After equilibration, the temperature in the equilibrium cell was measured and then vapor and liquid samples were withdrawn with a 1 mL Hamilton Sample Lock syringe and after that injected into the cooled 2 mL autosampler vial containing approximately 1 mL of *o*-xylene solvent (used as a diluent). The compositions of both samples were immediately measured by gas chromatography (GC). To prevent spreading of the unpleasant odor of the sulfur compounds, the GC was placed in a closed and ventilated cupboard.

The liquid and vapor samples were analyzed with Agilent 6850A gas chromatograph equipped with an auto sampler and a flame ionization detector (FID). The GC-column used was a HP-1 dimethylpolysiloxane (60.0 m × 250 μm × 1.0 μm). The injector and FID were set at 250 °C. Helium was used as the carrier gas at a constant flow rate of 1 $\text{mL}\cdot\text{min}^{-1}$ and inlet split ratio 100:1. The initial oven temperature was held at 70 °C for 2 min and then increased subsequently to 150 °C at rate of 8 °C min^{-1} and was held at 150 °C for 3 min. The total run time was 15 min.

The pure components were used to determine the retention times, after that the GC was calibrated with 10 mixtures of known composition that were prepared gravimetrically. To reduce the

Table 3. Physical Properties of Pure Compounds[a]

	DMDS	butane	2-methylpropane	2-methylpropene	*trans*-but-2-ene	ethanol	ETBE
CAS Registry No.[b]	624-92-0	106-97-8	75-28-5	115-11-7	624-64-6	64-17-5	637-92-3
T_C/K	606[c]	425.12[d]	407.8[d]	417.9[d]	428.6[d]	514[d]	509.4[d]
p_C/MPa	5.36[c]	3.80[d]	3.60[d]	4.00[d]	4.10[d]	6.137[d]	2.934[d]
ω	0.265[c]	0.200164[d]	0.183521[d]	0.19484[d]	0.217592[d]	0.634[d]	0.3162[d]
v_i/cm^3·mol	89.118[c]	101.394[d]	105.35[d]	95.3646[d]	93.6136[d]	58.62[d]	138.8[d]
A[e]	7.1352[f]					9.988[g]	7.0796[h]
B[e]	3080.0182[f]					3803.989[g]	2766.9942[h]
C[e]	−55.7933[f]					−41.535[g]	−50.5078[h]
T_{min}	332.19					300.40	312.51
T_{max}	382.02					345.10	345.90
$\lvert\Delta P^S_{\text{aver}}\rvert$ [i]/kPa	0.2					0.1	0.0

[a] Critical temperature, T_C, critical pressure, p_C, acentric factor, ω, molar volume v_i at 298 K. [b] Supplied by author. [c] Reference 4. [d] Reference 5. [e] $P^S/\text{MPa} = \exp(A - [B/(T/\text{K} + C)])$. [f] Reference 19. [g] Reference 20. [h] Reference 21. [i] $\lvert\Delta P^S_{\text{aver}}\rvert = (\sum_{i=1}^{N}\lvert P_{i,\text{calc}} - P_{i,\text{exp}}\rvert)/N$.

volume of the sample, the solvent was added. The response factor F_2 of component 2 was determined with eq 1.

$$\frac{m_2}{m_1}\frac{A_1}{A_2} = F_2 \qquad (1)$$

Therefore, the vapor or liquid composition of component 1 can be calculated from

$$x_1 = \frac{\dfrac{A_1}{M_1}}{\dfrac{A_1}{M_1} + \left(F_2\dfrac{A_2}{M_2}\right)} \qquad (2)$$

where A_1 and A_2 are the GC peak areas, M_1 and M_2 are the molar masses, and m_1 and m_2 are masses in the gravimetrically prepared sample of components 1 and 2, respectively. The maximum error of liquid and vapor composition measurements is estimated to be 0.003 in mole fraction.

Data Reduction. *Thermodynamic Model.* The activity coefficients were calculated from

$$\gamma_i = \frac{y_i P \phi_i}{x_i P_i^s \phi_i^s}\exp\int_P^{P_i^s}\frac{V_i^L}{RT}\,dP \qquad (3)$$

where y_i is the mole fraction of component i in the vapor phase, P is the total pressure of the system, ϕ_i is the fugacity coefficient of component i in the vapor phase, x_i is mole fraction of the component i in the liquid phase, P_i^S is the vapor pressure of pure component i at the system temperature, ϕ_i^S is the pure component-saturated liquid fugacity coefficient at the system temperature T, V_i^L is the molar volume of pure component i in liquid phase at the system temperature, T is temperature in Kelvin, and R is the universal gas constant (8.314 41 J·K^{-1}·mol^{-1}).

The Soave−Redlich−Kwong equation of state with quadratic mixing rules in the attractive parameter and linear in covolume was used for vapor-phase fugacity coefficient calculation.[10] The binary interaction parameter in the quadratic mixing rules was set to zero. The Rackett equation[11] was used to calculate the liquid molar volume in the Poynting factor. Compound properties used in the data reduction are shown in Table 3.

Static Total Pressure Method. The data measured in the static total pressure 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 reduced by the Legendre polynomials as the liquid activity coefficient model.[12] The data reduction was performed according to the Barker method.[13] The amount of parameters for Legendre polynomials[12] was increased until the average absolute deviation of pressure 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 the in-house software, VLEFIT.[14] The data reduction was also made with the Wilson model[15] as the activity coefficient model. The objective function (OF) used in the barker method is presented in eq 4, where N_{VLE} is the number of points used in the fit.

$$\text{OF} = \frac{1}{N_{\text{VLE}}}\sum_{i=1}^{N_{\text{VLE}}}\frac{\lvert p_{i,\,\text{calc}} - p_{i,\,\text{meas}}\rvert}{p_{i,\,\text{meas}}} \qquad (4)$$

Circulation Still Measurements. Also these measurements were processed with VLEFIT software.[14] The Antoine parameters for vapor pressure and other properties used in the calculations are presented in Table 2.

The liquid-phase activity coefficients of all systems studied were correlated with the Wilson[15] model. The objective function (OF) used for fitting of the activity coefficient model parameters is given by eq 5, where N_{VLE} is the number of points used in the fit.

$$\text{OF} = \frac{1}{N_{\text{VLE}}}\sum_{k=1}^{N_{\text{VLE}}}\sum_{i=1}^{2}\frac{\lvert \gamma^k_{i,\,\text{calc}} - \gamma^k_{i,\,\text{exp}}\rvert}{\gamma^k_{i,\,\text{exp}}} \qquad (5)$$

Error Analysis of the Static Total Pressure Measurements. Maximum uncertainty in the liquid density correlation was estimated as the maximum absolute error between the data sets used to obtain the correlation and the corresponding calculated value at temperatures from (270 to 310) K. The maximum error in density was 0.30% for butane, 0.28% for 2-methylpropane, 0.15% for 2-methylpropene, 0.76% for *trans*-but-2-ene, and 0.06% for DMDS. Uncertainty in the injection volume was ±0.02 cm^3, obtained from calibration experiments with distilled water. Uncertainty in the temperature of the pump was ±0.1 K, and uncertainty in the pressure of the pump was ±20 kPa, which affected the uncertainty in the density and the uncertainty in the compressibility of the liquid inside the pump. Uncertainty in the cell temperature measurements was estimated to be ±0.03 K. Uncertainty in the cell pressure measurement was ±0.4 kPa. Uncertainty in the reduced data depended on the uncertainty in the measured values of the temperature, the pressure, and the overall molar composition. Maximum theoretical error of the

Table 4. VLE Data for Butane (1) + DMDS (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
350.36 ± 0.03	0.3536 ± 0.0014	0.0000 ± 0.0000	1.0000 ± 0.0000	951.7 ± 0.4	951.7 ± 0.4	1.0000 ± 1.0000	1.0000 ± 0.0000	1.00 ± 0.00	2.83 ± 0.03
350.36 ± 0.03	0.3536 ± 0.0014	0.0166 ± 0.0002	0.9553 ± 0.0008	905.7 ± 0.4	905.5 ± 1.0	0.9526 ± 0.0009	0.9934 ± 0.0002	1.00 ± 0.00	2.53 ± 0.02
350.36 ± 0.03	0.3536 ± 0.0014	0.0194 ± 0.0002	0.9480 ± 0.0008	898.7 ± 0.4	898.5 ± 1.0	0.9450 ± 0.0009	0.9925 ± 0.0002	1.00 ± 0.00	2.49 ± 0.02
350.38 ± 0.03	0.3536 ± 0.0014	0.0401 ± 0.0003	0.8981 ± 0.0010	854.1 ± 0.4	854.2 ± 1.0	0.8930 ± 0.0010	0.9864 ± 0.0003	1.01 ± 0.00	2.23 ± 0.01
350.38 ± 0.03	0.3536 ± 0.0014	0.0639 ± 0.0003	0.8469 ± 0.0011	813.3 ± 0.4	813.4 ± 0.9	0.8403 ± 0.0012	0.9811 ± 0.0004	1.03 ± 0.00	2.02 ± 0.01
350.38 ± 0.03	0.3536 ± 0.0014	0.0901 ± 0.0003	0.7969 ± 0.0012	777.2 ± 0.4	777.3 ± 0.8	0.7895 ± 0.0013	0.9765 ± 0.0005	1.05 ± 0.00	1.84 ± 0.01
350.38 ± 0.03	0.3536 ± 0.0014	0.1190 ± 0.0003	0.7481 ± 0.0013	744.4 ± 0.4	744.6 ± 0.6	0.7404 ± 0.0013	0.9724 ± 0.0005	1.08 ± 0.00	1.70 ± 0.01
350.37 ± 0.03	0.3536 ± 0.0014	0.1529 ± 0.0004	0.6981 ± 0.0013	712.6 ± 0.4	712.6 ± 0.5	0.6904 ± 0.0014	0.9685 ± 0.0005	1.11 ± 0.00	1.58 ± 0.00
350.37 ± 0.03	0.3536 ± 0.0014	0.1928 ± 0.0004	0.6471 ± 0.0014	681.4 ± 0.4	681.3 ± 0.5	0.6398 ± 0.0014	0.9646 ± 0.0005	1.15 ± 0.00	1.48 ± 0.00
350.39 ± 0.03	0.3536 ± 0.0014	0.2391 ± 0.0004	0.5966 ± 0.0014	651.3 ± 0.4	651.2 ± 0.6	0.5901 ± 0.0014	0.9607 ± 0.0006	1.19 ± 0.00	1.39 ± 0.00
350.39 ± 0.03	0.3536 ± 0.0014	0.2920 ± 0.0005	0.5477 ± 0.0014	621.6 ± 0.4	621.4 ± 0.7	0.5421 ± 0.0014	0.9568 ± 0.0006	1.24 ± 0.00	1.32 ± 0.00
350.38 ± 0.03	0.3536 ± 0.0014	0.3557 ± 0.0006	0.4985 ± 0.0013	590.9 ± 0.4	590.5 ± 0.7	0.4941 ± 0.0014	0.9527 ± 0.0007	1.30 ± 0.00	1.26 ± 0.00
350.38 ± 0.03	0.3554 ± 0.0014	0.3570 ± 0.0006	0.4989 ± 0.0013	590.4 ± 0.4	590.7 ± 0.7	0.4946 ± 0.0014	0.9528 ± 0.0007	1.30 ± 0.00	1.26 ± 0.00
350.38 ± 0.03	0.2917 ± 0.0011	0.3570 ± 0.0006	0.4497 ± 0.0014	556.1 ± 0.4	556.4 ± 0.6	0.4436 ± 0.0014	0.9479 ± 0.0007	1.36 ± 0.00	1.20 ± 0.00
350.38 ± 0.03	0.2370 ± 0.0010	0.3570 ± 0.0006	0.3990 ± 0.0014	518.6 ± 0.4	518.6 ± 0.5	0.3911 ± 0.0014	0.9421 ± 0.0008	1.44 ± 0.01	1.15 ± 0.00
350.38 ± 0.03	0.1916 ± 0.0008	0.3570 ± 0.0006	0.3493 ± 0.0013	478.2 ± 0.4	478.2 ± 0.5	0.3398 ± 0.0014	0.9353 ± 0.0009	1.54 ± 0.01	1.11 ± 0.00
350.38 ± 0.03	0.1515 ± 0.0007	0.3570 ± 0.0006	0.2980 ± 0.0013	432.4 ± 0.4	432.3 ± 0.6	0.2872 ± 0.0013	0.9263 ± 0.0010	1.64 ± 0.01	1.08 ± 0.00
350.38 ± 0.03	0.1188 ± 0.0006	0.3570 ± 0.0006	0.2497 ± 0.0012	384.5 ± 0.4	384.5 ± 0.6	0.2382 ± 0.0012	0.9150 ± 0.0011	1.76 ± 0.01	1.06 ± 0.00
350.38 ± 0.03	0.0893 ± 0.0005	0.3570 ± 0.0006	0.2000 ± 0.0011	329.5 ± 0.4	329.6 ± 0.5	0.1885 ± 0.0011	0.8985 ± 0.0013	1.89 ± 0.01	1.03 ± 0.00
350.38 ± 0.03	0.0637 ± 0.0004	0.3570 ± 0.0006	0.1515 ± 0.0010	269.8 ± 0.4	269.8 ± 0.7	0.1408 ± 0.0010	0.8733 ± 0.0014	2.04 ± 0.02	1.02 ± 0.00
350.38 ± 0.03	0.0411 ± 0.0003	0.3570 ± 0.0006	0.1032 ± 0.0009	203.2 ± 0.4	203.2 ± 0.7	0.0944 ± 0.0009	0.8286 ± 0.0017	2.21 ± 0.03	1.01 ± 0.00
350.38 ± 0.03	0.0204 ± 0.0003	0.3570 ± 0.0006	0.0540 ± 0.0008	127.9 ± 0.4	128.0 ± 0.5	0.0485 ± 0.0008	0.7231 ± 0.0026	2.39 ± 0.04	1.00 ± 0.00
350.38 ± 0.03	0.0126 ± 0.0002	0.3570 ± 0.0006	0.0341 ± 0.0007	95.5 ± 0.4	95.3 ± 0.7	0.0304 ± 0.0007	0.6256 ± 0.0042	2.48 ± 0.04	1.00 ± 0.00
350.38 ± 0.03	0.0057 ± 0.0002	0.3570 ± 0.0006	0.0159 ± 0.0006	63.9 ± 0.4	64.0 ± 1.1	0.0140 ± 0.0006	0.4402 ± 0.0089	2.55 ± 0.05	1.00 ± 0.00
350.38 ± 0.03	0.0000 ± 0.0000	0.3570 ± 0.0006	0.0000 ± 0.0000	36.0 ± 0.4	36.0 ± 0.4	0.0000 ± 0.0000	0.0000 ± 0.0000	2.63 ± 0.05	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.

Table 5. VLE Data for 2-Methylpropane (1) + DMDS (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
350.54 ± 0.03	0.3410 ± 0.0037	0.0000 ± 0.0000	1.0000 ± 0.0000	1269.5 ± 0.4	1269.5 ± 0.4	1.0000 ± 0.0000	1.0000 ± 0.0000	1.00 ± 0.00	3.31 ± 0.07
350.54 ± 0.03	0.3410 ± 0.0037	0.0027 ± 0.0002	0.9921 ± 0.0008	1257.0 ± 0.4	1256.6 ± 1.3	0.9913 ± 0.0008	0.9987 ± 0.0002	1.00 ± 0.00	3.23 ± 0.06
350.54 ± 0.03	0.3410 ± 0.0037	0.0103 ± 0.0002	0.9706 ± 0.0010	1223.4 ± 0.4	1223.3 ± 1.4	0.9679 ± 0.0011	0.9955 ± 0.0003	1.00 ± 0.00	3.02 ± 0.05
350.55 ± 0.03	0.3410 ± 0.0037	0.0180 ± 0.0002	0.9498 ± 0.0012	1194.0 ± 0.4	1193.6 ± 1.5	0.9454 ± 0.0014	0.9927 ± 0.0003	1.00 ± 0.00	2.84 ± 0.04
350.55 ± 0.03	0.3410 ± 0.0037	0.0380 ± 0.0003	0.8998 ± 0.0016	1131.0 ± 0.4	1130.4 ± 1.6	0.8922 ± 0.0019	0.9871 ± 0.0005	1.02 ± 0.00	2.48 ± 0.02
350.56 ± 0.03	0.3410 ± 0.0037	0.0612 ± 0.0003	0.8478 ± 0.0020	1074.5 ± 0.4	1074.1 ± 1.5	0.8381 ± 0.0023	0.9824 ± 0.0006	1.04 ± 0.00	2.20 ± 0.02
350.55 ± 0.03	0.3410 ± 0.0037	0.0868 ± 0.0003	0.7971 ± 0.0023	1025.5 ± 0.4	1025.4 ± 1.2	0.7861 ± 0.0027	0.9786 ± 0.0006	1.06 ± 0.00	1.98 ± 0.01
350.55 ± 0.03	0.3410 ± 0.0037	0.1162 ± 0.0003	0.7459 ± 0.0026	981.0 ± 0.4	981.0 ± 0.8	0.7344 ± 0.0029	0.9752 ± 0.0006	1.09 ± 0.00	1.80 ± 0.01
350.55 ± 0.03	0.3410 ± 0.0037	0.1481 ± 0.0004	0.6972 ± 0.0028	941.5 ± 0.4	941.6 ± 0.5	0.6858 ± 0.0031	0.9722 ± 0.0006	1.13 ± 0.01	1.66 ± 0.00
350.55 ± 0.03	0.3410 ± 0.0037	0.1859 ± 0.0004	0.6472 ± 0.0030	902.8 ± 0.4	902.9 ± 0.7	0.6364 ± 0.0033	0.9694 ± 0.0006	1.17 ± 0.01	1.54 ± 0.00
350.55 ± 0.03	0.3410 ± 0.0037	0.2304 ± 0.0004	0.5968 ± 0.0031	864.5 ± 0.4	864.5 ± 0.9	0.5871 ± 0.0033	0.9666 ± 0.0006	1.23 ± 0.01	1.44 ± 0.00
350.54 ± 0.03	0.3410 ± 0.0037	0.2820 ± 0.0005	0.5474 ± 0.0031	827.0 ± 0.4	826.7 ± 0.9	0.5391 ± 0.0033	0.9637 ± 0.0006	1.28 ± 0.01	1.36 ± 0.00
350.55 ± 0.03	0.3410 ± 0.0037	0.3431 ± 0.0005	0.4985 ± 0.0031	789.1 ± 0.4	788.2 ± 0.9	0.4919 ± 0.0033	0.9608 ± 0.0007	1.35 ± 0.01	1.29 ± 0.00
350.54 ± 0.03	0.3438 ± 0.0037	0.3473 ± 0.0005	0.4975 ± 0.0031	786.8 ± 0.4	787.3 ± 0.9	0.4911 ± 0.0033	0.9607 ± 0.0007	1.35 ± 0.01	1.29 ± 0.00
350.54 ± 0.03	0.2809 ± 0.0031	0.3473 ± 0.0005	0.4471 ± 0.0031	740.8 ± 0.4	741.3 ± 0.8	0.4380 ± 0.0033	0.9571 ± 0.0007	1.43 ± 0.01	1.22 ± 0.00
350.55 ± 0.03	0.2284 ± 0.0025	0.3473 ± 0.0005	0.3968 ± 0.0031	691.3 ± 0.4	691.5 ± 0.6	0.3850 ± 0.0032	0.9528 ± 0.0008	1.53 ± 0.01	1.17 ± 0.00
350.55 ± 0.03	0.1847 ± 0.0021	0.3473 ± 0.0005	0.3472 ± 0.0029	637.5 ± 0.4	637.4 ± 0.8	0.3331 ± 0.0031	0.9476 ± 0.0009	1.64 ± 0.01	1.12 ± 0.00
350.54 ± 0.03	0.1481 ± 0.0017	0.3473 ± 0.0005	0.2990 ± 0.0028	579.1 ± 0.4	579.1 ± 0.9	0.2832 ± 0.0029	0.9413 ± 0.0010	1.76 ± 0.02	1.09 ± 0.00
350.55 ± 0.03	0.1145 ± 0.0014	0.3473 ± 0.0005	0.2480 ± 0.0025	510.1 ± 0.4	509.9 ± 0.7	0.2311 ± 0.0027	0.9321 ± 0.0011	1.91 ± 0.02	1.06 ± 0.00
350.54 ± 0.03	0.0866 ± 0.0011	0.3473 ± 0.0005	0.1997 ± 0.0023	436.3 ± 0.4	436.3 ± 0.4	0.1828 ± 0.0023	0.9196 ± 0.0011	2.06 ± 0.03	1.04 ± 0.00
350.54 ± 0.03	0.0614 ± 0.0008	0.3473 ± 0.0005	0.1502 ± 0.0019	351.8 ± 0.4	352.1 ± 0.8	0.1348 ± 0.0020	0.8993 ± 0.0012	2.25 ± 0.04	1.02 ± 0.00
350.54 ± 0.03	0.0392 ± 0.0006	0.3473 ± 0.0005	0.1014 ± 0.0015	259.3 ± 0.4	259.3 ± 1.0	0.0890 ± 0.0016	0.8620 ± 0.0015	2.45 ± 0.05	1.01 ± 0.00
350.55 ± 0.03	0.0191 ± 0.0004	0.3473 ± 0.0005	0.0521 ± 0.0011	156.2 ± 0.4	156.0 ± 0.6	0.0446 ± 0.0011	0.7692 ± 0.0025	2.67 ± 0.07	1.00 ± 0.00
350.54 ± 0.03	0.0118 ± 0.0003	0.3473 ± 0.0005	0.0328 ± 0.0009	112.7 ± 0.4	112.8 ± 0.9	0.0278 ± 0.0009	0.6805 ± 0.0041	2.77 ± 0.08	1.00 ± 0.00
350.54 ± 0.03	0.0021 ± 0.0002	0.3473 ± 0.0005	0.0061 ± 0.0006	51.0 ± 0.4	50.7 ± 1.6	0.0051 ± 0.0006	0.2885 ± 0.0191	2.90 ± 0.10	1.00 ± 0.00
350.55 ± 0.03	0.0000 ± 0.0000	0.3473 ± 0.0005	0.0000 ± 0.0000	36.1 ± 0.4	36.1 ± 0.4	0.0000 ± 0.0000	0.0000 ± 0.0000	2.93 ± 0.10	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.

Table 6. VLE Data for 2-Methylpropene (1) + DMDS (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
350.43 ± 0.03	0.3765 ± 0.0009	0.0000 ± 0.0000	1.0000 ± 0.0000	1154.3 ± 0.4	1154.3 ± 0.4	1.0000 ± 0.0000	1.0000 ± 0.0000	1.00 ± 0.00	2.38 ± 0.02
350.44 ± 0.03	0.3765 ± 0.0009	0.0032 ± 0.0002	0.9916 ± 0.0006	1143.1 ± 0.4	1142.6 ± 1.1	0.9910 ± 0.0007	0.9990 ± 0.0001	1.00 ± 0.00	2.33 ± 0.02
350.43 ± 0.03	0.3765 ± 0.0009	0.0117 ± 0.0002	0.9699 ± 0.0007	1113.5 ± 0.4	1112.5 ± 1.1	0.9677 ± 0.0007	0.9966 ± 0.0001	1.00 ± 0.00	2.21 ± 0.01
350.43 ± 0.03	0.3765 ± 0.0009	0.0203 ± 0.0002	0.9489 ± 0.0007	1086.5 ± 0.4	1085.3 ± 1.2	0.9453 ± 0.0008	0.9944 ± 0.0002	1.00 ± 0.00	2.11 ± 0.01
350.43 ± 0.03	0.3765 ± 0.0009	0.0417 ± 0.0003	0.9003 ± 0.0008	1028.9 ± 0.4	1027.9 ± 1.2	0.8943 ± 0.0008	0.9899 ± 0.0002	1.01 ± 0.00	1.91 ± 0.01
350.44 ± 0.03	0.3765 ± 0.0009	0.0662 ± 0.0003	0.8505 ± 0.0008	976.3 ± 0.4	975.7 ± 1.1	0.8429 ± 0.0009	0.9859 ± 0.0003	1.03 ± 0.00	1.74 ± 0.01
350.44 ± 0.03	0.3765 ± 0.0009	0.0955 ± 0.0003	0.7976 ± 0.0009	924.7 ± 0.4	924.6 ± 0.9	0.7891 ± 0.0010	0.9820 ± 0.0003	1.05 ± 0.00	1.60 ± 0.01
350.43 ± 0.03	0.3765 ± 0.0009	0.1274 ± 0.0003	0.7472 ± 0.0010	878.6 ± 0.4	878.8 ± 0.7	0.7384 ± 0.0010	0.9785 ± 0.0004	1.07 ± 0.00	1.49 ± 0.01
350.43 ± 0.03	0.3765 ± 0.0009	0.1630 ± 0.0004	0.6979 ± 0.0010	835.7 ± 0.4	836.1 ± 0.6	0.6893 ± 0.0010	0.9752 ± 0.0004	1.09 ± 0.00	1.41 ± 0.00
350.43 ± 0.03	0.3765 ± 0.0009	0.2051 ± 0.0004	0.6473 ± 0.0010	792.7 ± 0.4	793.1 ± 0.7	0.6394 ± 0.0010	0.9717 ± 0.0004	1.13 ± 0.00	1.33 ± 0.00
350.43 ± 0.03	0.3765 ± 0.0009	0.2542 ± 0.0005	0.5970 ± 0.0010	750.4 ± 0.4	750.4 ± 0.9	0.5900 ± 0.0010	0.9681 ± 0.0005	1.16 ± 0.00	1.27 ± 0.00
350.43 ± 0.03	0.3765 ± 0.0009	0.3110 ± 0.0005	0.5477 ± 0.0010	709.0 ± 0.4	708.2 ± 1.0	0.5419 ± 0.0010	0.9643 ± 0.0005	1.20 ± 0.00	1.22 ± 0.00
350.43 ± 0.03	0.3765 ± 0.0009	0.3803 ± 0.0006	0.4975 ± 0.0010	666.6 ± 0.4	664.2 ± 1.0	0.4932 ± 0.0010	0.9600 ± 0.0006	1.24 ± 0.00	1.17 ± 0.00
350.43 ± 0.03	0.3769 ± 0.0009	0.3794 ± 0.0006	0.4984 ± 0.0010	666.1 ± 0.4	664.9 ± 1.0	0.4941 ± 0.0010	0.9601 ± 0.0006	1.24 ± 0.00	1.18 ± 0.00
350.43 ± 0.03	0.3089 ± 0.0008	0.3794 ± 0.0006	0.4488 ± 0.0010	616.4 ± 0.4	616.2 ± 0.8	0.4427 ± 0.0010	0.9550 ± 0.0006	1.29 ± 0.00	1.14 ± 0.00
350.43 ± 0.03	0.2516 ± 0.0007	0.3794 ± 0.0006	0.3987 ± 0.0010	564.6 ± 0.4	564.9 ± 0.5	0.3910 ± 0.0010	0.9489 ± 0.0007	1.34 ± 0.00	1.10 ± 0.00
350.43 ± 0.03	0.2035 ± 0.0006	0.3794 ± 0.0006	0.3492 ± 0.0010	511.2 ± 0.4	511.4 ± 0.6	0.3400 ± 0.0010	0.9414 ± 0.0008	1.40 ± 0.00	1.08 ± 0.00
350.43 ± 0.03	0.1617 ± 0.0005	0.3794 ± 0.0006	0.2988 ± 0.0010	454.1 ± 0.4	454.1 ± 0.8	0.2886 ± 0.0010	0.9318 ± 0.0010	1.46 ± 0.00	1.05 ± 0.00
350.44 ± 0.03	0.1272 ± 0.0004	0.3794 ± 0.0006	0.2512 ± 0.0009	396.7 ± 0.4	396.8 ± 0.9	0.2405 ± 0.0009	0.9196 ± 0.0011	1.53 ± 0.01	1.04 ± 0.00
350.43 ± 0.03	0.0938 ± 0.0004	0.3794 ± 0.0006	0.1982 ± 0.0009	329.2 ± 0.4	329.2 ± 0.8	0.1877 ± 0.0009	0.9002 ± 0.0013	1.61 ± 0.01	1.02 ± 0.00
350.43 ± 0.03	0.0670 ± 0.0003	0.3794 ± 0.0006	0.1500 ± 0.0008	263.9 ± 0.4	264.0 ± 0.6	0.1405 ± 0.0008	0.8725 ± 0.0015	1.70 ± 0.01	1.01 ± 0.00
350.44 ± 0.03	0.0427 ± 0.0003	0.3794 ± 0.0006	0.1012 ± 0.0008	194.2 ± 0.4	194.2 ± 0.8	0.0936 ± 0.0008	0.8227 ± 0.0017	1.79 ± 0.02	1.01 ± 0.00
350.44 ± 0.03	0.0215 ± 0.0003	0.3794 ± 0.0006	0.0535 ± 0.0007	122.1 ± 0.4	122.0 ± 0.5	0.0489 ± 0.0007	0.7119 ± 0.0028	1.89 ± 0.03	1.00 ± 0.00
350.43 ± 0.03	0.0132 ± 0.0002	0.3794 ± 0.0006	0.0336 ± 0.0006	90.5 ± 0.4	90.5 ± 0.8	0.0305 ± 0.0006	0.6090 ± 0.0045	1.93 ± 0.04	1.00 ± 0.00
350.43 ± 0.03	0.0053 ± 0.0002	0.3794 ± 0.0006	0.0137 ± 0.0006	58.3 ± 0.4	58.3 ± 1.1	0.0123 ± 0.0006	0.3887 ± 0.0101	1.98 ± 0.04	1.00 ± 0.00
350.43 ± 0.03	0.0000 ± 0.0000	0.3794 ± 0.0006	0.0000 ± 0.0000	35.8 ± 0.4	35.8 ± 0.4	0.0000 ± 0.000	0.0000 ± 0.0000	2.01 ± 0.05	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.

Table 7. VLE Data for *trans*-But-2-ene (1) + DMDS (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
350.30 ± 0.03	0.3826 ± 0.0032	0.0000 ± 0.0000	1.0000 ± 0.0000	929.2 ± 0.4	928.9 ± 0.4	1.0000 ± 0.0000	1.0000 ± 0.0000	1.00 ± 0.00	2.28 ± 0.05
350.31 ± 0.03	0.3826 ± 0.0032	0.0041 ± 0.0002	0.9895 ± 0.0007	918.1 ± 0.4	917.9 ± 1.0	0.9888 ± 0.0007	0.9987 ± 0.0001	1.00 ± 0.00	2.23 ± 0.04
350.32 ± 0.03	0.3826 ± 0.0032	0.0122 ± 0.0002	0.9690 ± 0.0008	897.3 ± 0.4	897.2 ± 1.0	0.9673 ± 0.0009	0.9962 ± 0.0002	1.00 ± 0.00	2.13 ± 0.03
350.32 ± 0.03	0.3826 ± 0.0032	0.0210 ± 0.0002	0.9481 ± 0.0010	877.2 ± 0.4	876.9 ± 1.1	0.9453 ± 0.0011	0.9938 ± 0.0003	1.00 ± 0.00	2.05 ± 0.03
350.32 ± 0.03	0.3826 ± 0.0032	0.0438 ± 0.0003	0.8972 ± 0.0013	831.3 ± 0.4	831.2 ± 1.0	0.8926 ± 0.0015	0.9884 ± 0.0004	1.01 ± 0.00	1.86 ± 0.02
350.31 ± 0.03	0.3826 ± 0.0032	0.0693 ± 0.0003	0.8466 ± 0.0016	790.1 ± 0.4	789.8 ± 0.9	0.8408 ± 0.0018	0.9837 ± 0.0005	1.02 ± 0.00	1.71 ± 0.01
350.32 ± 0.03	0.3826 ± 0.0032	0.0981 ± 0.0003	0.7959 ± 0.0019	751.8 ± 0.4	751.7 ± 0.7	0.7894 ± 0.0020	0.9793 ± 0.0005	1.04 ± 0.00	1.59 ± 0.01
350.32 ± 0.03	0.3826 ± 0.0032	0.1295 ± 0.0003	0.7471 ± 0.0021	716.8 ± 0.4	716.8 ± 0.6	0.7404 ± 0.0022	0.9752 ± 0.0006	1.06 ± 0.00	1.49 ± 0.01
350.31 ± 0.03	0.3826 ± 0.0032	0.1659 ± 0.0004	0.6976 ± 0.0023	682.3 ± 0.4	682.4 ± 0.5	0.6910 ± 0.0024	0.9711 ± 0.0006	1.09 ± 0.00	1.40 ± 0.00
350.31 ± 0.03	0.3826 ± 0.0032	0.2085 ± 0.0004	0.6473 ± 0.0024	648.2 ± 0.4	648.3 ± 0.6	0.6411 ± 0.0025	0.9669 ± 0.0006	1.12 ± 0.00	1.33 ± 0.00
350.31 ± 0.03	0.3826 ± 0.0032	0.2579 ± 0.0005	0.5973 ± 0.0025	614.4 ± 0.4	614.4 ± 0.6	0.5920 ± 0.0026	0.9626 ± 0.0007	1.15 ± 0.01	1.27 ± 0.00
350.31 ± 0.03	0.3826 ± 0.0032	0.3160 ± 0.0005	0.5476 ± 0.0025	580.5 ± 0.4	580.4 ± 0.6	0.5432 ± 0.0026	0.9580 ± 0.0007	1.19 ± 0.01	1.22 ± 0.00
350.31 ± 0.03	0.3826 ± 0.0032	0.3835 ± 0.0006	0.4994 ± 0.0025	546.9 ± 0.4	546.5 ± 0.5	0.4960 ± 0.0026	0.9530 ± 0.0008	1.22 ± 0.01	1.18 ± 0.00
350.32 ± 0.03	0.3878 ± 0.0033	0.3994 ± 0.0006	0.4926 ± 0.0025	541.2 ± 0.4	541.8 ± 0.5	0.4896 ± 0.0025	0.9523 ± 0.0008	1.23 ± 0.01	1.17 ± 0.00
350.32 ± 0.03	0.3170 ± 0.0027	0.3994 ± 0.0006	0.4425 ± 0.0025	502.8 ± 0.4	503.1 ± 0.5	0.4381 ± 0.0025	0.9461 ± 0.0009	1.28 ± 0.01	1.14 ± 0.00
350.32 ± 0.03	0.2581 ± 0.0022	0.3994 ± 0.0006	0.3925 ± 0.0024	462.6 ± 0.4	462.6 ± 0.6	0.3869 ± 0.0025	0.9387 ± 0.0010	1.33 ± 0.01	1.10 ± 0.00
350.31 ± 0.03	0.2090 ± 0.0019	0.3994 ± 0.0006	0.3436 ± 0.0023	420.8 ± 0.4	420.6 ± 0.7	0.3368 ± 0.0024	0.9299 ± 0.0011	1.39 ± 0.01	1.08 ± 0.00
350.31 ± 0.03	0.1671 ± 0.0015	0.3994 ± 0.0006	0.295 ± 0.0022	376.8 ± 0.4	376.5 ± 0.7	0.2874 ± 0.0023	0.9188 ± 0.0013	1.45 ± 0.01	1.06 ± 0.00
350.32 ± 0.03	0.1310 ± 0.0012	0.3994 ± 0.0006	0.2470 ± 0.0020	330.5 ± 0.4	330.3 ± 0.6	0.2391 ± 0.0021	0.9044 ± 0.0014	1.52 ± 0.01	1.04 ± 0.00
350.32 ± 0.03	0.0998 ± 0.0010	0.3994 ± 0.0006	0.1999 ± 0.0018	281.9 ± 0.4	281.9 ± 0.4	0.1920 ± 0.0019	0.8846 ± 0.0015	1.60 ± 0.02	1.02 ± 0.00
350.32 ± 0.03	0.0731 ± 0.0008	0.3994 ± 0.0006	0.1547 ± 0.0016	232.3 ± 0.4	232.5 ± 0.6	0.1474 ± 0.0016	0.8563 ± 0.0017	1.68 ± 0.02	1.01 ± 0.00
350.32 ± 0.03	0.0480 ± 0.0006	0.3994 ± 0.0006	0.1072 ± 0.0013	176.6 ± 0.4	177.0 ± 0.7	0.1012 ± 0.0013	0.8062 ± 0.0021	1.77 ± 0.03	1.01 ± 0.00
350.31 ± 0.03	0.0269 ± 0.0004	0.3994 ± 0.0006	0.0631 ± 0.0010	121.5 ± 0.4	121.7 ± 0.6	0.0589 ± 0.0010	0.7117 ± 0.0030	1.87 ± 0.04	1.00 ± 0.00
350.32 ± 0.03	0.0154 ± 0.0003	0.3994 ± 0.0006	0.0371 ± 0.0008	87.6 ± 0.4	87.5 ± 0.8	0.0345 ± 0.0008	0.5941 ± 0.0048	1.93 ± 0.04	1.00 ± 0.00
350.31 ± 0.03	0.0092 ± 0.0003	0.3994 ± 0.0006	0.0225 ± 0.0007	67.6 ± 0.4	67.6 ± 0.9	0.0208 ± 0.0007	0.4706 ± 0.0072	1.96 ± 0.05	1.00 ± 0.00
350.30 ± 0.03	0.0000 ± 0.0000	0.3994 ± 0.0006	0.0000 ± 0.0000	36.1 ± 0.4	36.1 ± 0.4	0.0000 ± 0.0000	0.0000 ± 0.0000	2.02 ± 0.05	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).

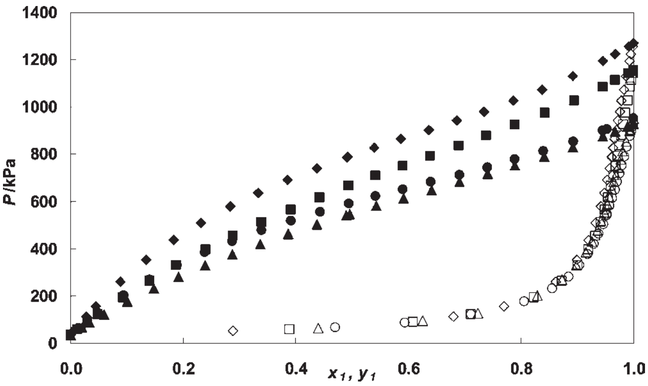

Figure 2. Experimental pressure and liquid- and vapor-phase mole fractions at 350 K of DMDS (2) + butane, *x* ●, *y* ○; + 2-methylpropane, *x* ◆, *y* ◇; + 2-methylpropene, *x* ■, *y* □; + *trans*-but-2-ene, *x* ▲, *y* △.

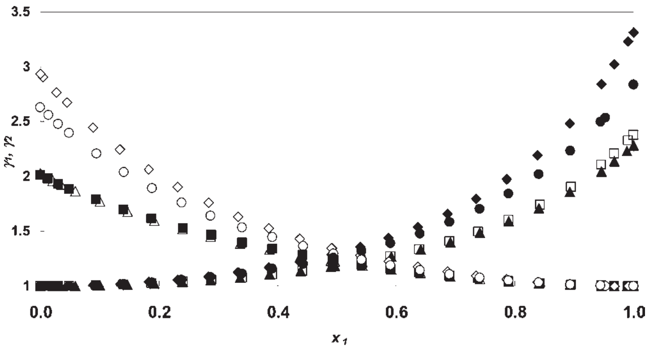

Figure 3. Activity coefficients at 350 K: (○) butane (1) + (●) DMDS system; (◇) 2-methylpropane (1) + (◆) DMDS system; (■) 2-methylpropene (1) + (□) DMDS system; (△) *trans*-but-2-ene (1) + (▲) DMDS system.

Table 8. Isothermal VLE Measurements at 343.15 K, Liquid-Phase (x_1) and Vapor-Phase (y_1) Mole Fractions, Pressure (P), and Activity Coefficient (γ_i), for Systems DMDS (1) + Ethanol (2) and DMDS (1) + ETBE (2)

DMDS (1) + ethanol (2) at 343.15 K					DMDS (1) + ETBE (2) at 343.15 K				
x_1	y_1	P/kPa	γ_1	γ_2	x_1	y_1	P/kPa	γ_1	γ_2
0.000	0.000	72.5		1.00	0.000	0.000	92.9		1.00
0.031	0.053	74.4	4.53	1.00	0.093	0.044	88.2	1.47	1.00
0.072	0.105	76.1	3.91	1.01	0.207	0.096	82.4	1.35	1.02
0.141	0.164	77.4	3.19	1.04	0.332	0.156	75.9	1.26	1.04
0.233	0.214	77.6	2.52	1.09	0.461	0.221	69.0	1.17	1.08
0.325	0.246	77.0	2.06	1.18	0.582	0.292	62.0	1.11	1.15
0.446	0.269	75.5	1.61	1.37	0.700	0.374	54.8	1.04	1.25
0.569	0.303	73.2	1.38	1.63	0.822	0.498	45.7	0.99	1.42
0.720	0.344	68.5	1.16	2.22	0.894	0.624	39.7	0.99	1.55
0.825	0.396	62.9	1.07	3.00	0.944	0.760	34.6	1.00	1.64
0.911	0.498	52.8	1.03	4.12	0.974	0.873	31.0	1.00	1.70
0.962	0.658	40.6	1.00	5.11	1.000	1.000	27.8	1.00	
1.000	1.000	27.8	1.00						

overall molar composition was calculated by the method presented by Hynynen et al.[16] 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.[17,18]

■ RESULTS AND DISCUSSION

Static Total Pressure Measurements. 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 measured data, equilibrium-phase compositions, and compound activity coefficients are shown in Tables 4−7. Equilibrium-phase compositions are presented in Figure 2 and activity coefficient of the regressed C4 alkane and C4 alkene systems are presented in Figure 3. All measured binary systems showed a positive deviation from Raoult's law.

As the measured pure component vapor pressures were acceptable, both sides of measured binaries coincided, and the Legendre polynomials could describe the data with good accuracy. The data were considered to be of good quality.

Also 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 activity coefficient model were close to the ones obtained from the regression using the Legendre polynomials.

Circulation Still Measurements. Vapor pressure of dimethyl disulfide, ethanol, and ETBE were measured in previous studies.[19−21] These parameters with the recommended temperature range of the vapor pressure equations are presented in Table 2.

The isothermal VLE measurements (P, x_1, and y_1) and calculated activity coefficients are reported in Table 8. The $P-x_1-y_1$ diagrams are presented in Figure 4. The $\gamma_1-\gamma_2-x_1$ diagram is presented in Figure 5. All systems show positive deviation from Raoult's law. No azeotropic behavior was observed in system dimethyl disulfide + ETBE at 343.15 K. A maximum pressure azeotrope was found in the ethanol (1) + dimethyl disulfide (2) + system (azeotropic conditions: x_1 = 0.801, P = 78.1 kPa, T = 343.15 K).

Wilson interaction parameters with small lambda (λ_{12} and λ_{21}) and the average of the absolute deviations of pressure and vapor-phase composition in mole fraction for the measured

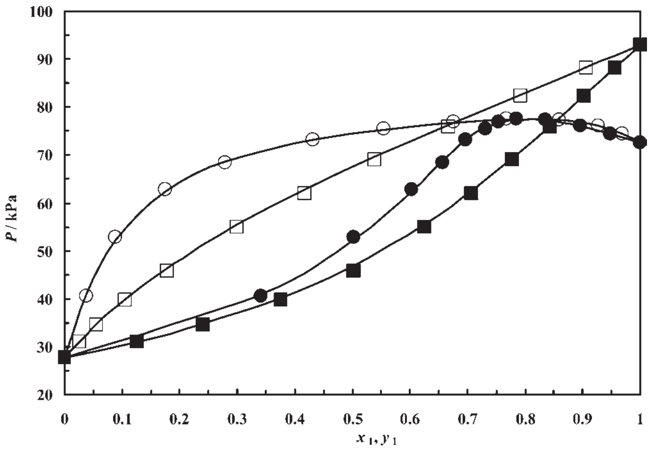

Figure 4. Experimental pressure and liquid- and vapor-phase equilibrium composition in mole fractions at K of DMDS (2) + ethanol, x ○, y ●; DMDS (2) + ETBE, x ■, y □; Wilson model, —.

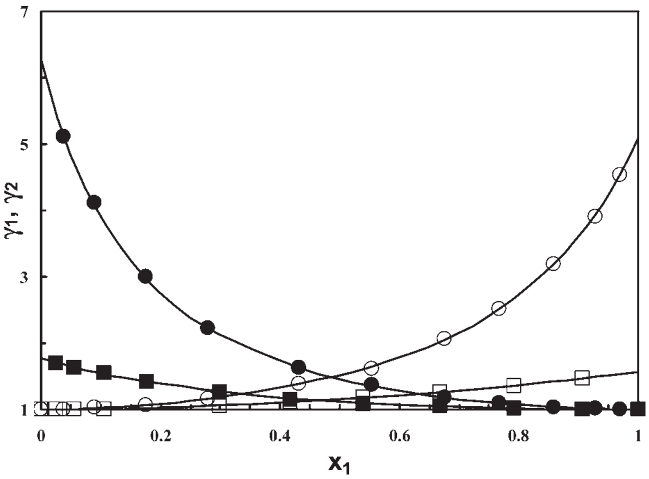

Figure 5. Activity coefficients at 350 K of (●) ethanol (1) + (○) DMDS system; (■) ETBE (1) + (□) DMDS system.

Table 9. Legendre Liquid Activity Coefficient Model Parameters (Legendre, $a_{i,j}$), Absolute Average Pressure Residuals ($|\Delta P|$), and Infinite Dilution Activity Coefficients ($\gamma_1^\infty, \gamma_2^\infty$), Wilson Liquid Activity Coefficient Model Parameters (Wilson $\lambda_{i,j}$), Absolute Average Vapor-Phase Composition Mole Fraction Residuals ($|\Delta y|$) at Temperature of Measurement (T)[a]

	system 1	system 2	system 3	system 4	system 5	system 6
	350 K	351 K	350 K	350 K	343 K	343 K
Legendre, $a_{0,0}$	0.986850	1.11305	0.759653	0.744936		
Legendre, $a_{1,0}$	0.0373437	0.0582667	0.0840095	0.0618308		
Legendre, $a_{2,0}$	0.0162596	0.0241948	0.0218635	0.0191669		
Legendre, $a_{3,0}$	0.000444541	0.00234212	−0.000385644	−0.00122994		
$|\Delta P|$/kPa	0.2	0.2	0.4	0.2		
Legendre $\gamma_1^\infty, \gamma_2^\infty$	2.63, 2.83	2.93, 3.31	2.01, 2.38	2.02, 2.28		
Wilson $\lambda_{1,2}$/K	123.212	129.109	41.3975	65.1284	567.97	34.487
Wilson $\lambda_{2,1}$/K	277.461	334.701	267.117	228.381	171.77	161.70
$|\Delta P|$/kPa	0.2	0.3	0.8	0.6	0.2	0.3
$|\Delta y|$					0.001	0.002
Wilson $\gamma_1^\infty, \gamma_2^\infty$	2.63, 2.84	2.95, 3.33	1.99, 2.37	1.99, 2.25	6.27, 5.10	1.77, 1.56

[a] System 1 (butane + DMDS), system 2 (2-methylpropane + DMDS), system 3 (2-methylpropene + DMDS), system 4 (*trans*-but-2-ene + DMDS), system 5 (ethanol + DMDS), system 6 (ETBE + DMDS).

systems are presented in Table 9. The averages of the absolute deviations for pressure and vapor-phase composition are small. Good agreement between measurements and model were achieved for the two systems measured. The activity coefficients at infinite dilution for all systems measured calculated from the Wilson model are also shown in Table 9.

The integral test,[12] infinite dilution test,[22] and point test[12] were applied to check the consistency of the measured VLE data. All systems measured with the circulation still passed the consistency tests applied.

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