Figure Captions

Figure 1 – Vapor pressure of methyl esters: **(A)** L: laurate (□, Rose and Supina [36]; ○, Scott et al., [37]); M: myristate (▲, Rose and Supina [36]; ●, Chen et al. [39]); P: palmitate (△, Hou et al. [40]; □, Rose and Supina [36]; ◆, Chen et al. [39]; ◆, Widegren and Bruno [46]); **(B)** S: stearate (△, Hou et al. [40]; □, Rose and Supina [36]; ◆, Widegren and Bruno [46]); Oa: oleate (▲, Rose and Schrodt [41]; ●, Scott et al. [37]); La: linoleate (□, Scott et al. [37]) and Ln: linolenate (○, Scott et al. [37]). Symbols are experimental and lines were calculated using the PC-SAFT model.

Figure 2 – Vapor pressure curves of ethyl esters: **(A)** L: laurate (△, Shigley et al. [44]; □, Silva et al. [43]); M: myristate (○, Silva et al. [43]; ◇, Tang et al. [45]); P: palmitate (○, Tang et al. [45]; △, Silva et al. [43]; ◆, Widegren and Bruno [46], ●, Silva et al. [53]); **(B)** S: stearate (△, Silva et al. [43]; ○ Shigley et al. [44]; ■, Widegren and Bruno [46]); Oa: oleate (□, Silva et al. [43]; ◇, Ledanois [47]; ▲ Silva et al. [53]) and La: linoleate (■, Silva et al. [43]). Symbols are experimental and lines were calculated using the PC-SAFT model.

Figure 3 – Density profile as a function of temperature for **(A)** methyl esters and **(B)** ethyl esters (L: laurate; M: myristate; P: palmitate; S: stearate; Oa: oleate; La: linoleate and Ln: linolenate (with 1, 2 and 3 double bonds, respectively). Experimental [48] PC-SAFT calculations.

Figure 4 – Temperatures-composition diagrams for the ethyl esters binary mixtures. **(A)** ethyl myristate + ethyl palmitate (○, 1.5 kPa; □, 1.0 kPa; △, 0.5 kPa [45]), , **(B)** ethyl palmitate + ethyl oleate (○, 5.3329 kPa; □, 9.3326 kPa [53]). Lines are representing predicted values (k_{ij} = 0) using both models (——, PC-SAFT; ----, PC-SAFT-JC).

Figure 5 – Temperatures-composition diagrams for the methyl esters binary mixtures. **(A)** methyl laurate + methyl myristate (○, 4.0 kPa; □, 6.67 kPa; △, 13.33 kPa [36]), **(B)** methyl myristate + methyl palmitate (○, 1.4 kPa; □, 1.0 kPa; △, 0.5 kPa [39]). Lines are representing predicted values (k_{ij} = 0) using both models (——, PC-SAFT; ----, PC-SAFT-JC).

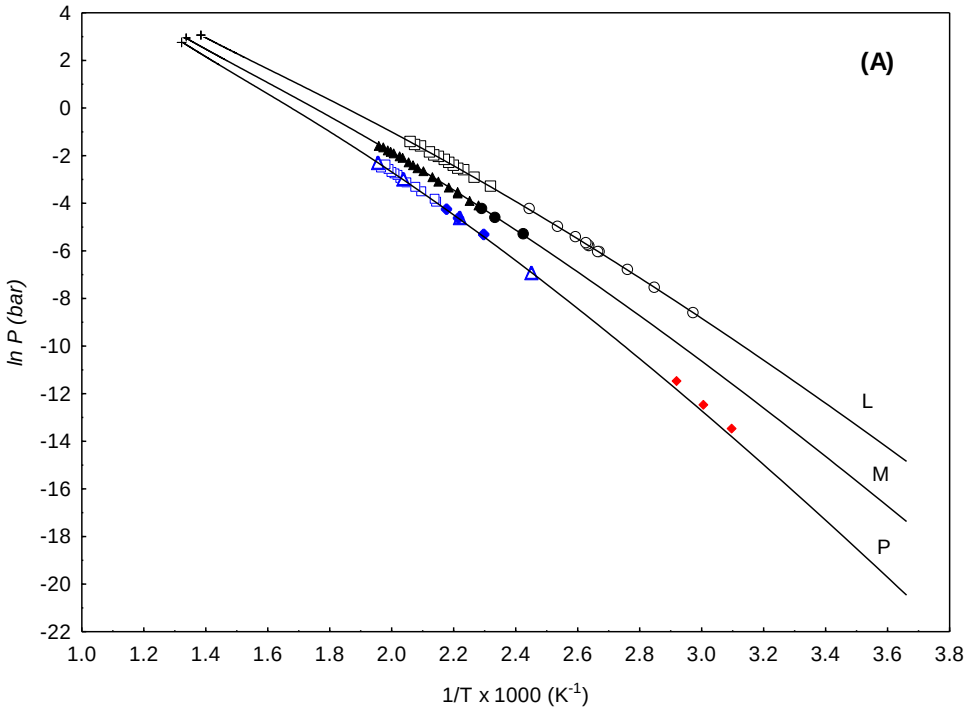
Figure 6 – Temperatures-composition diagrams for the methyl palmitate(1) + methyl stearate(2) system. Symbols are experimental data at different pressures (□, 0.5333 kPa [54]; ○, 3.947 kPa [36]; ◆, 10.0 kPa; ■, 5.0 kPa; ●, 1.0 kPa and ▲, 0.1 kPa [40]). Lines are the calculated values using both models (——, PC-SAFT; ----, PC-SAFT-JC) with k_{ij} = 0 **(A)** and k_{ij} = 0.01 **(B)**.

Figure 7 – Experimental and predicted melting points for ethyl esters: **(A)** (△, ethyl oleate(1) + ethyl laurate(2); □, ethyl palmitate(1) + ethyl laurate(2)) and **(B)** (●, ethyl linoleate(1) + ethyl palmitate(2); ○, ethyl oleate(1) + ethyl palmitate(2)). Calculated lines are the PC-SAFT model (k_{ij} = 0).

Figure 8 – VLE diagram for the systems ethanol(1) + hexyl acetate(2) and methanol(1) + hexyl acetate(2). Symbol are experimental data [58] and lines the PC-SAFT model using transferable cross-association parameters (k_{ij} = 0).

Figure 9 – Temperature-composition diagram for the systems **(A)** ethanol(1)+ethyl palmitate(2) and **(B)** ethanol(1)+ethyl stearate (2). Symbol are experimental data (△, 24 kPa; ○, 92 kPa [7]) and lines the PC-SAFT model using transferable cross-association parameters (——, PC-SAFT; ----, PC-SAFT-JC) with k_{ij} = 0.

Figure 10 – Pressure-composition diagram for the systems **(A)** ethanol(1) + ethyl laurate(2), **(B)** ethanol(1) + ethyl myristate(2), **(C)** methanol(1) + methyl laurate(2) and **(D)** methanol(1) + methyl myristate(2), at high temperatures. Symbol are experimental data (△, 493 K; □, 523 K; ○, 543 K, [60,61]) and lines are the calculated values using transferable cross-association parameters (——, PC-SAFT; ----, PC-SAFT-JC) with k_{ij} = 0.



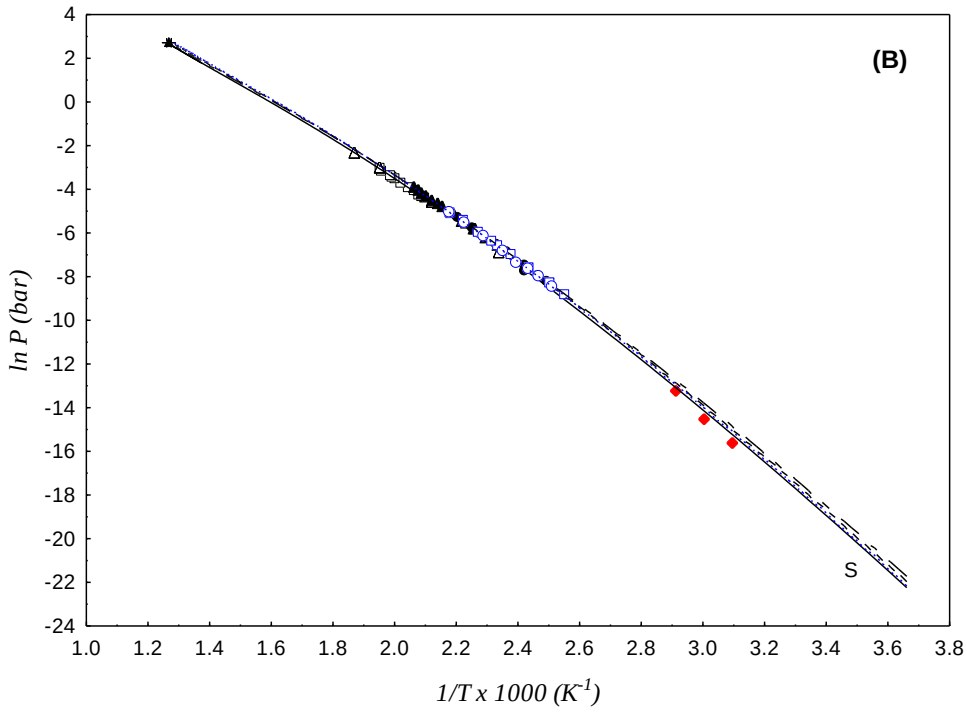
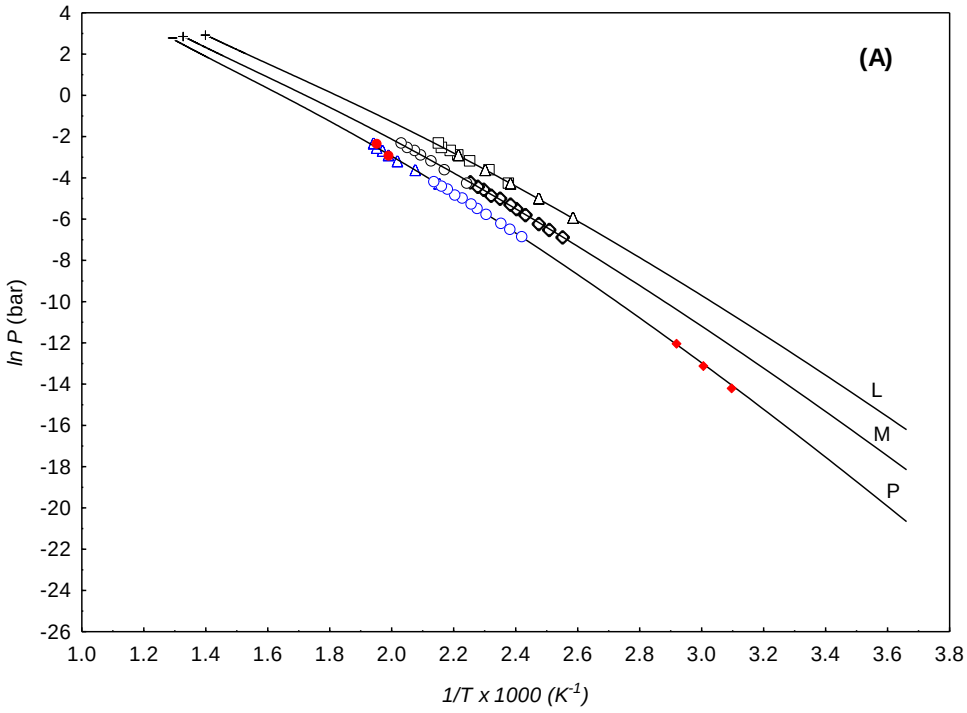


Figure 1



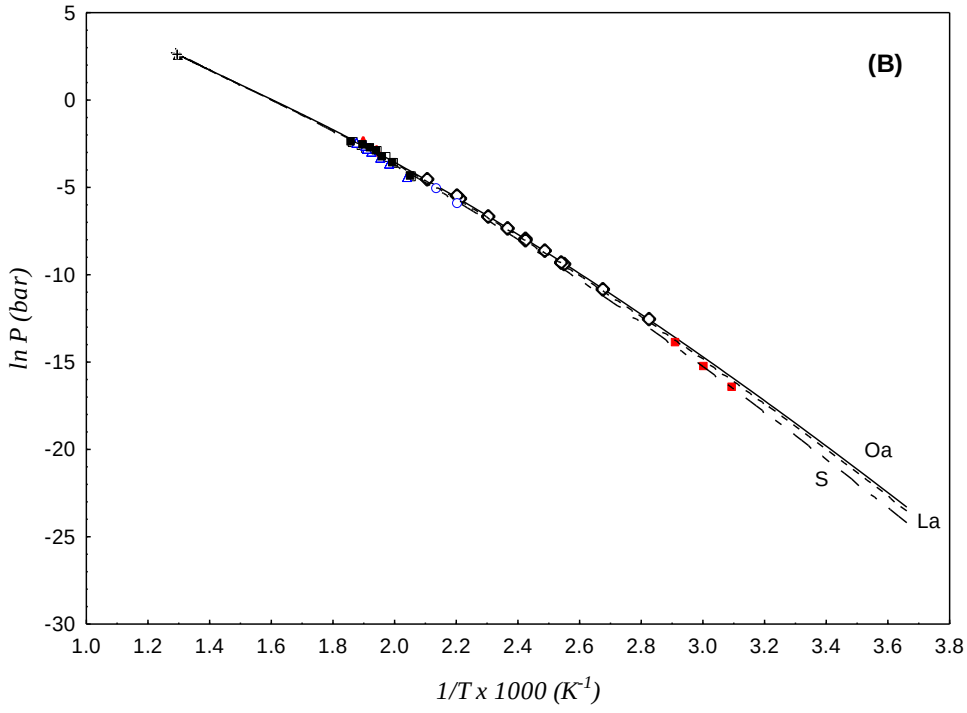
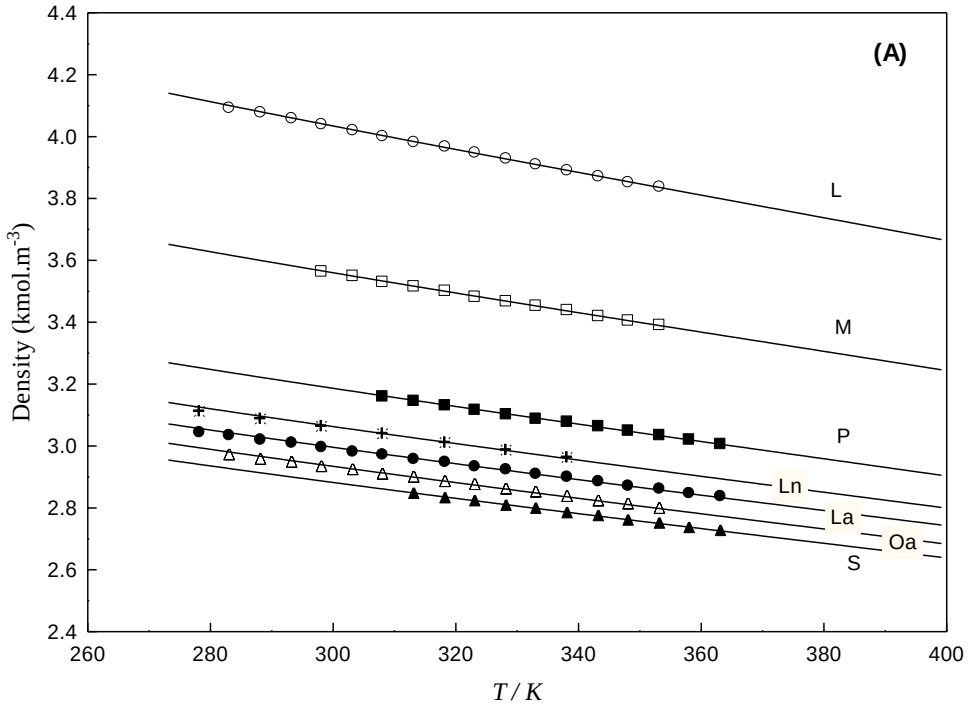


Figure 2


(A)
Density (kmol.m-3)
T / K
L
M
P
Ln
La
Oa
S

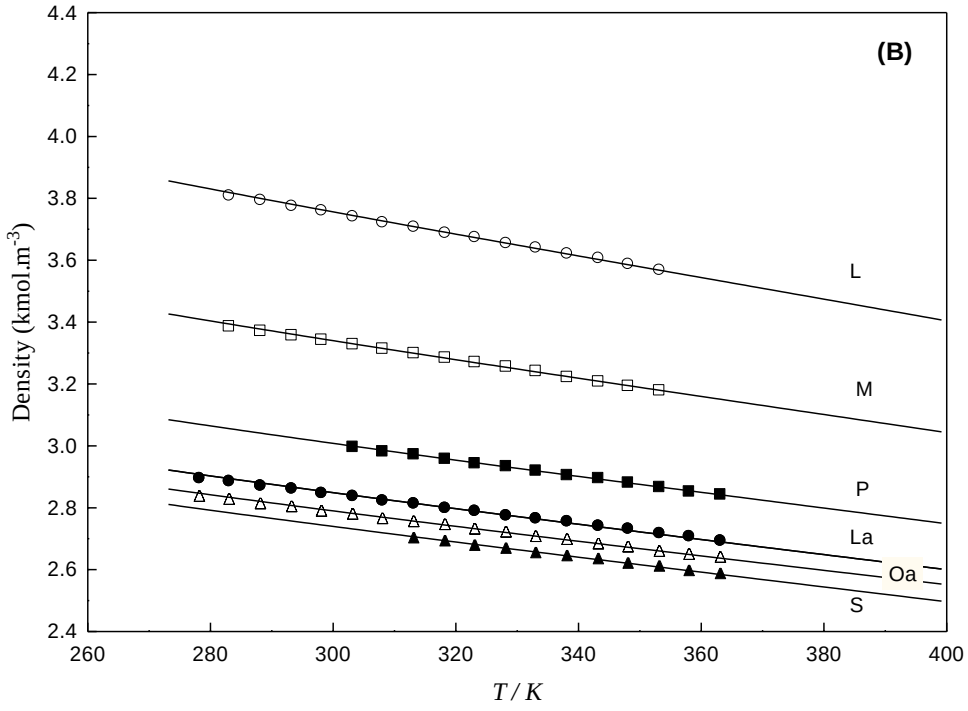
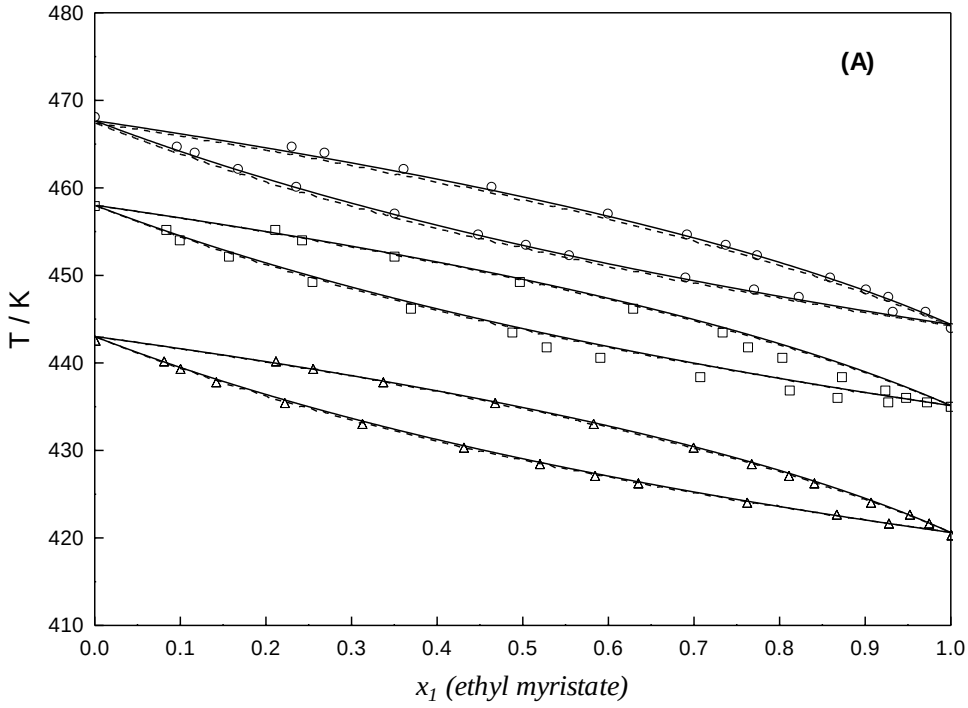

(B)
Density (kmol.m-3)
T / K
L
M
P
La
Oa
S

Figure 3


(A)
T / K
480
470
460
450
440
430
420
410
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
x1 (ethyl myristate)

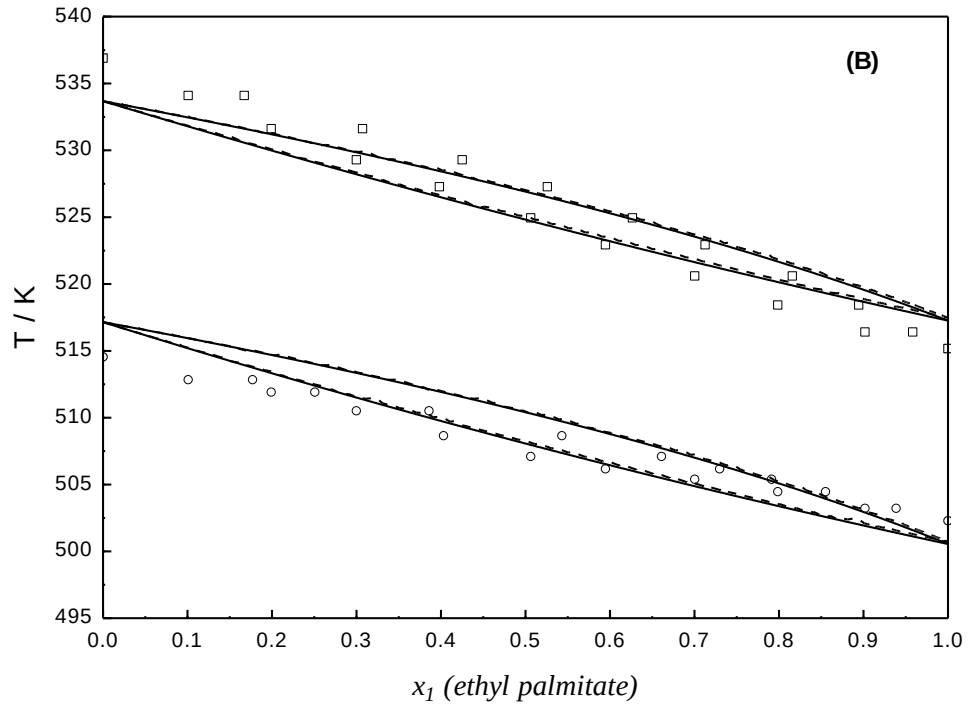
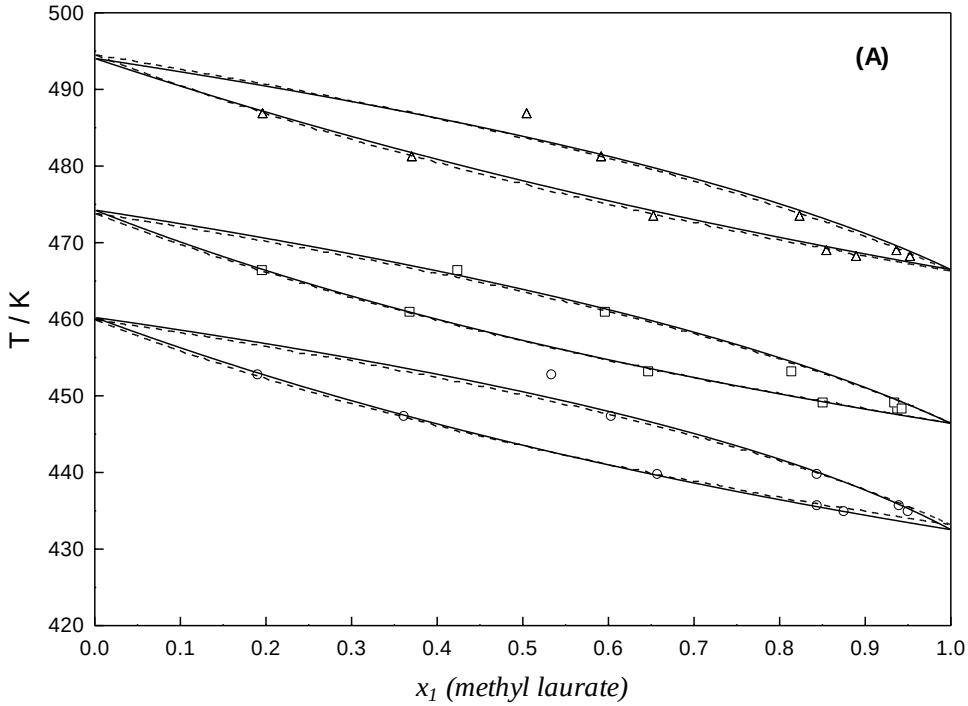

(B)
T / K
540
535
530
525
520
515
510
505
500
495
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
x1 (ethyl palmitate)

Figure 4


(A)
T / K
500
490
480
470
460
450
440
430
420
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
x1 (methyl laurate)

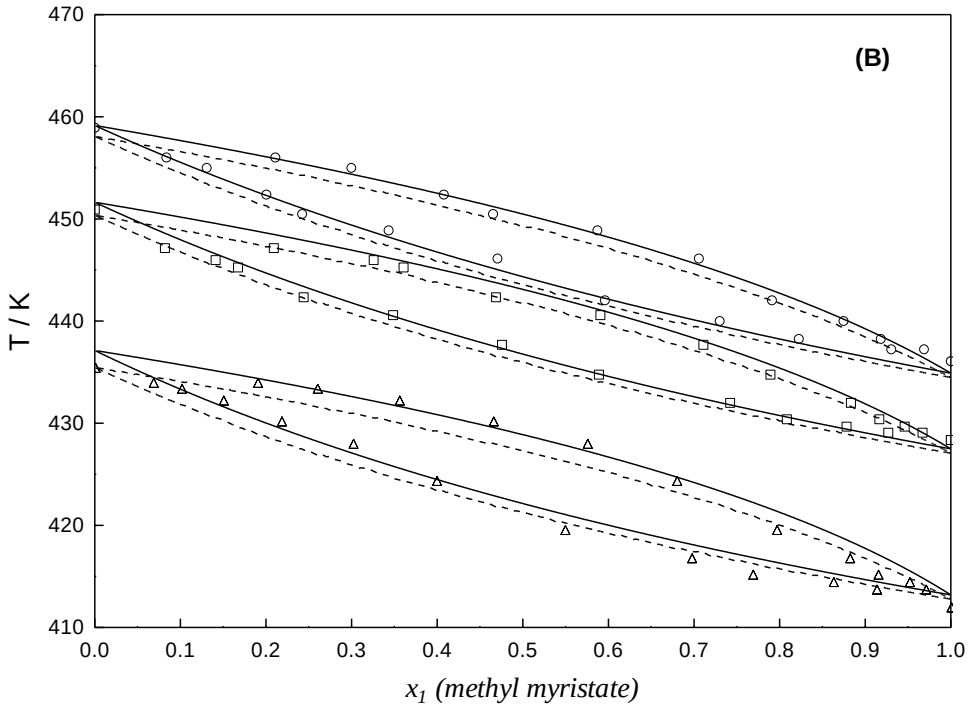
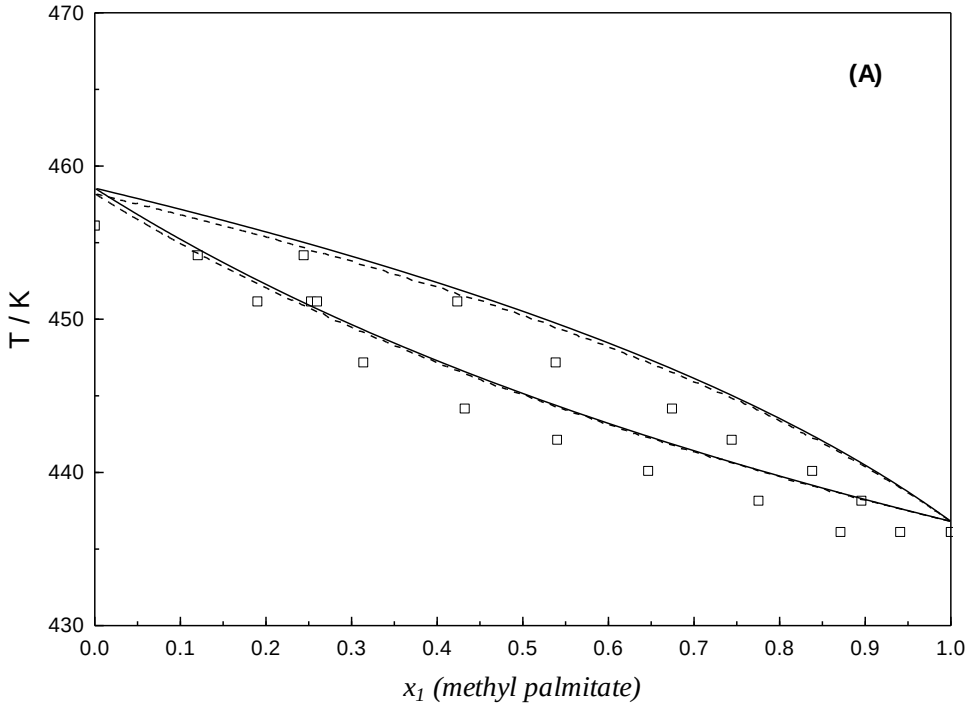

(B)
T / K
470
460
450
440
430
420
410
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
x1 (methyl myristate)

Figure 5


(A)
T / K
470
460
450
440
430
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
x_1 (methyl palmitate)

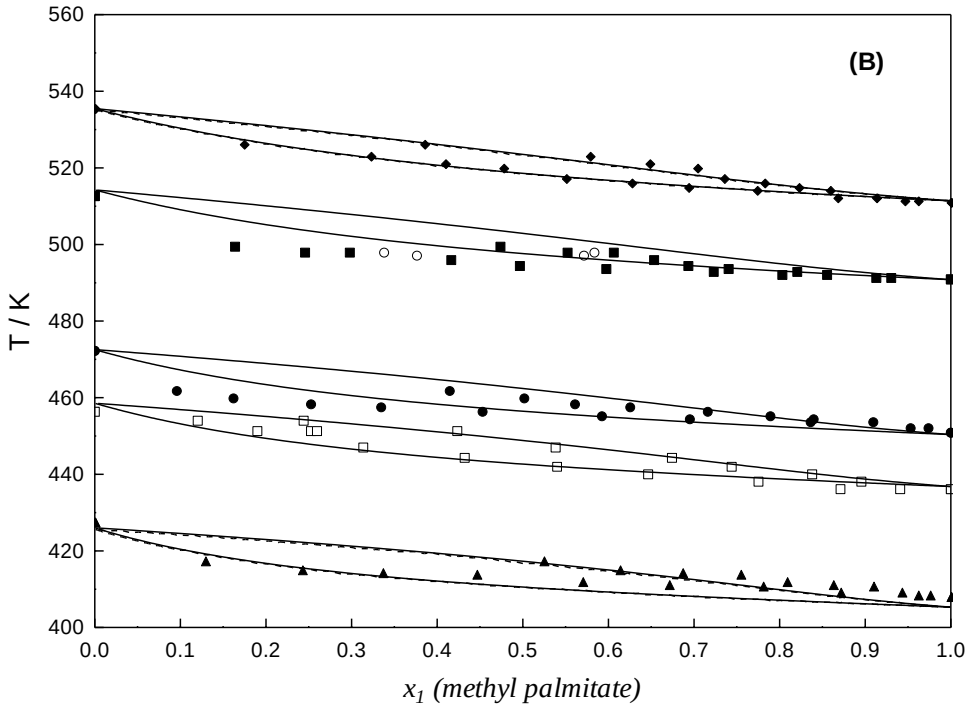

(B)
T / K
560
540
520
500
480
460
440
420
400
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
x_1 (methyl palmitate)

Figure 6

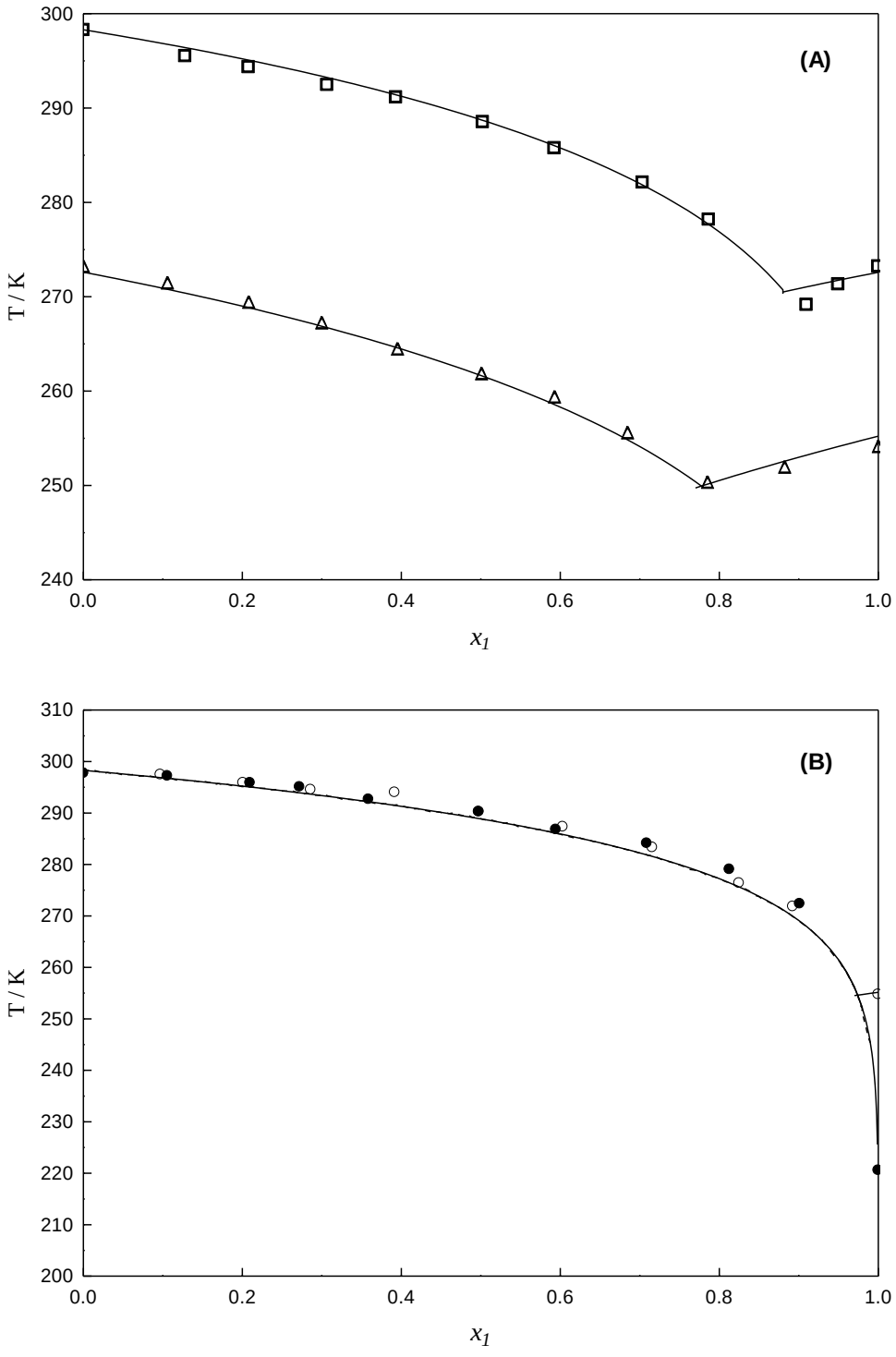
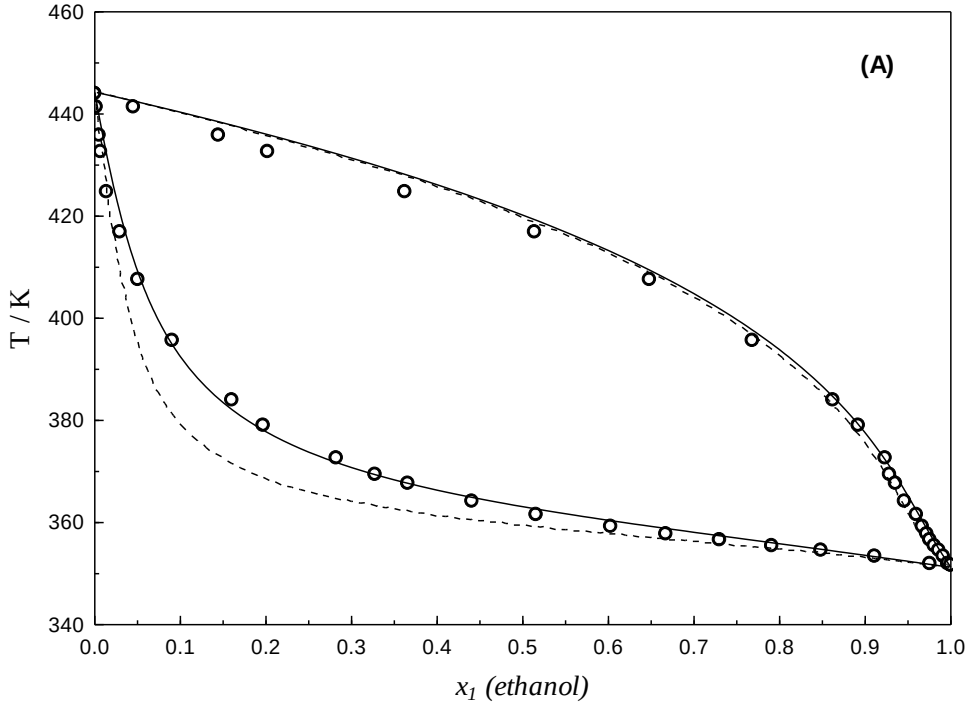


Figure 7


(A)
T / K
460
440
420
400
380
360
340
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
x_1 (ethanol)

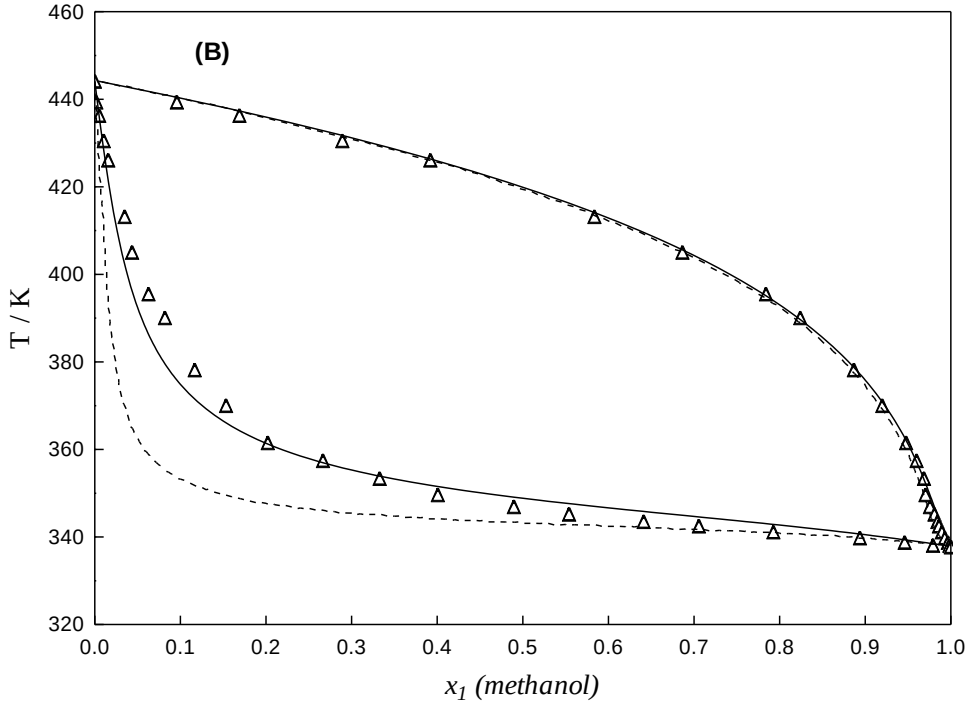
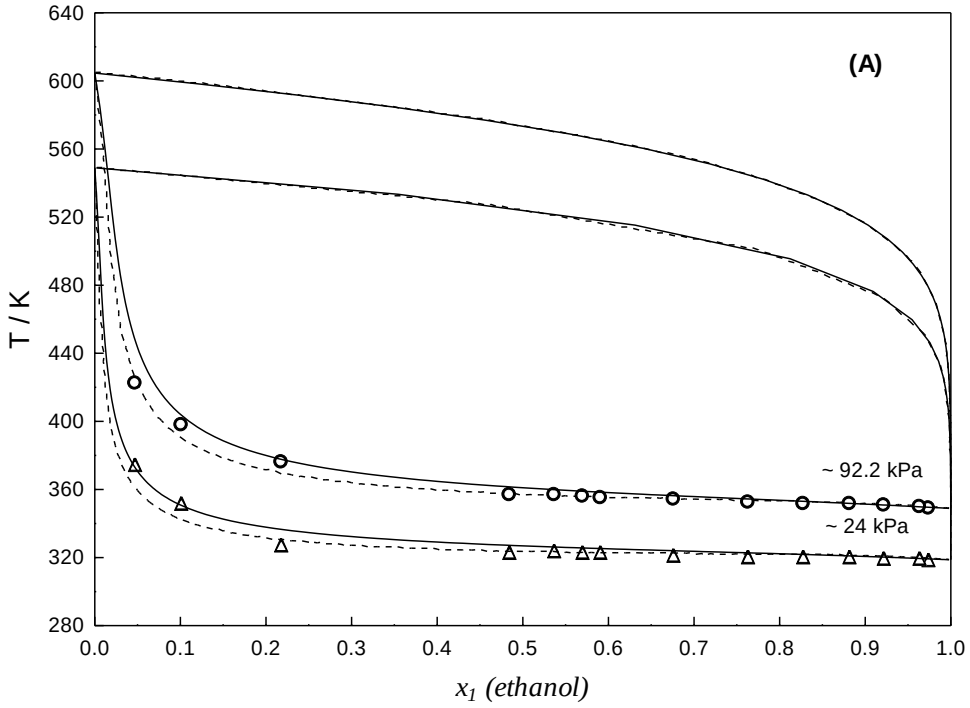

(B)
T / K
460
440
420
400
380
360
340
320
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
x_1 (methanol)

Figure 8


(A)
T / K
640
600
560
520
480
440
400
360
320
280
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
~ 92.2 kPa
~ 24 kPa
x1 (ethanol)

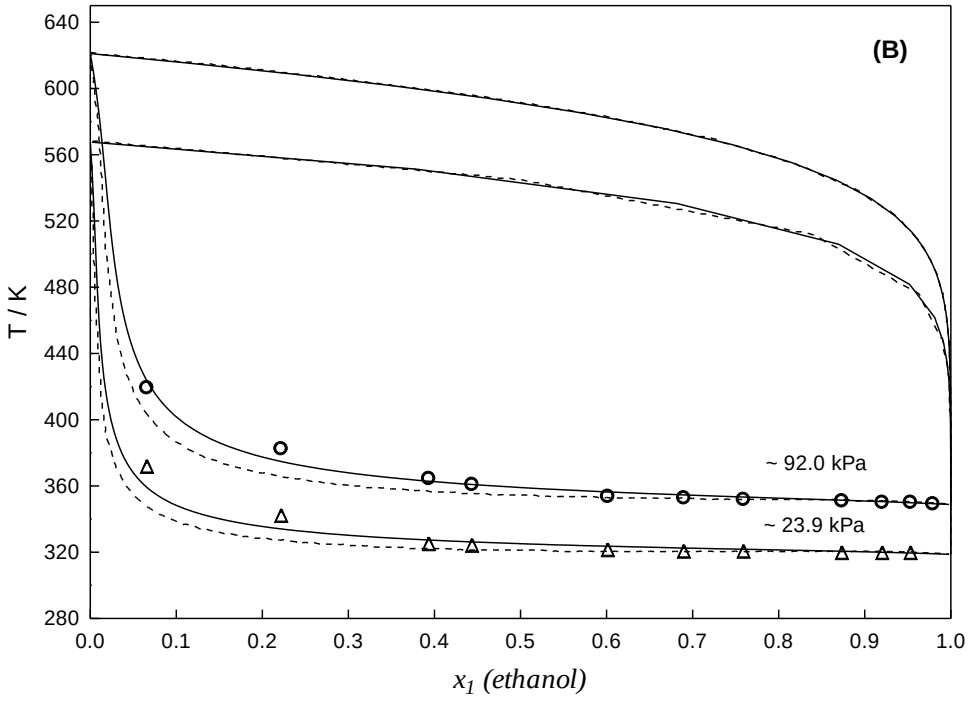
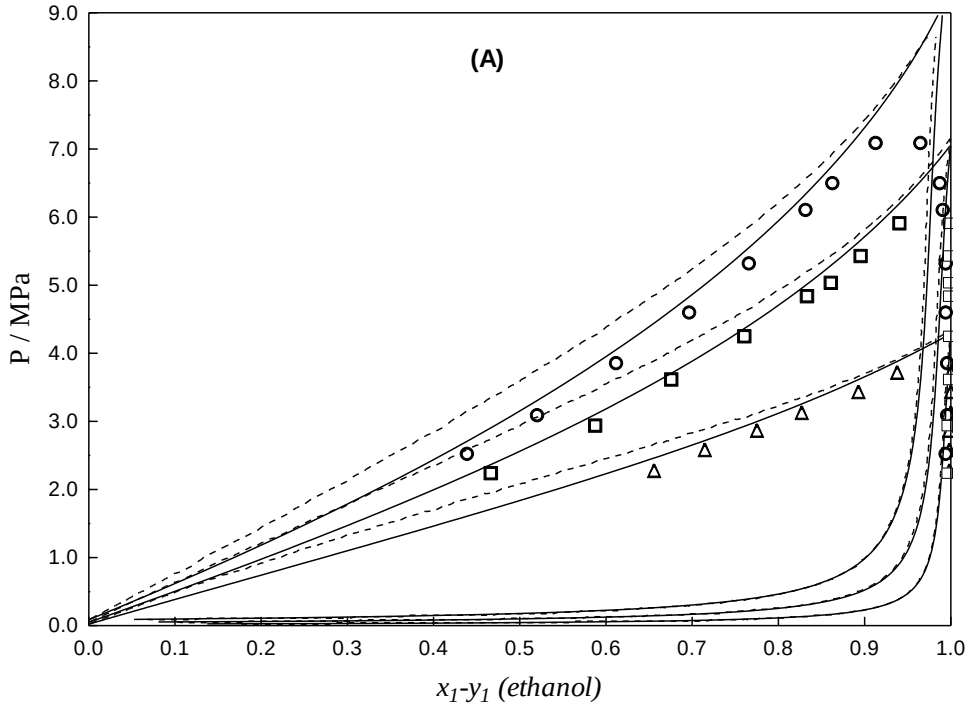
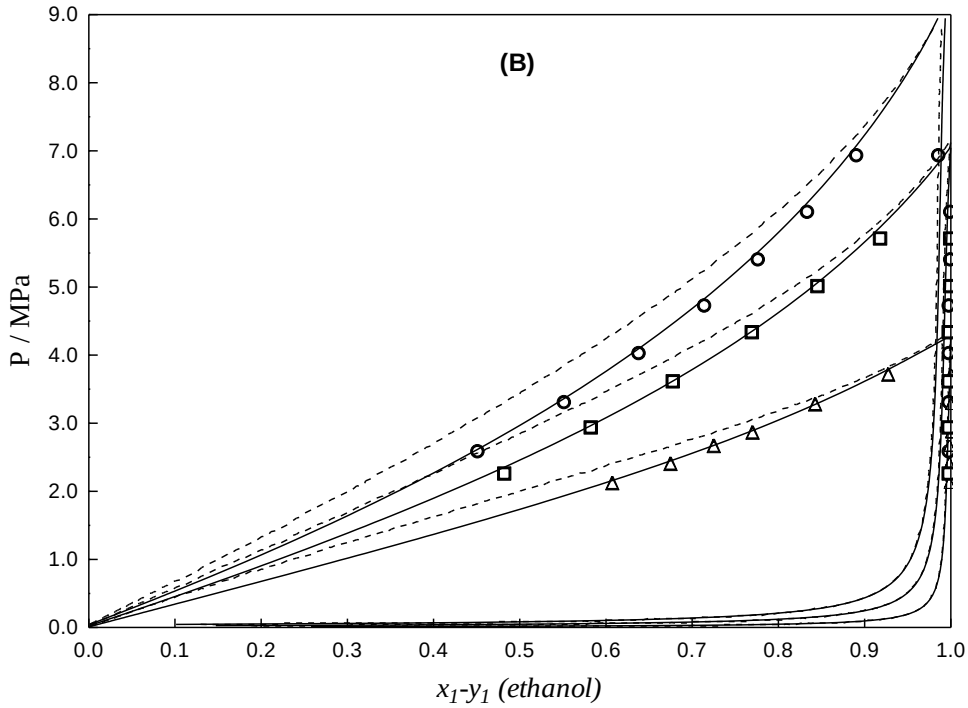
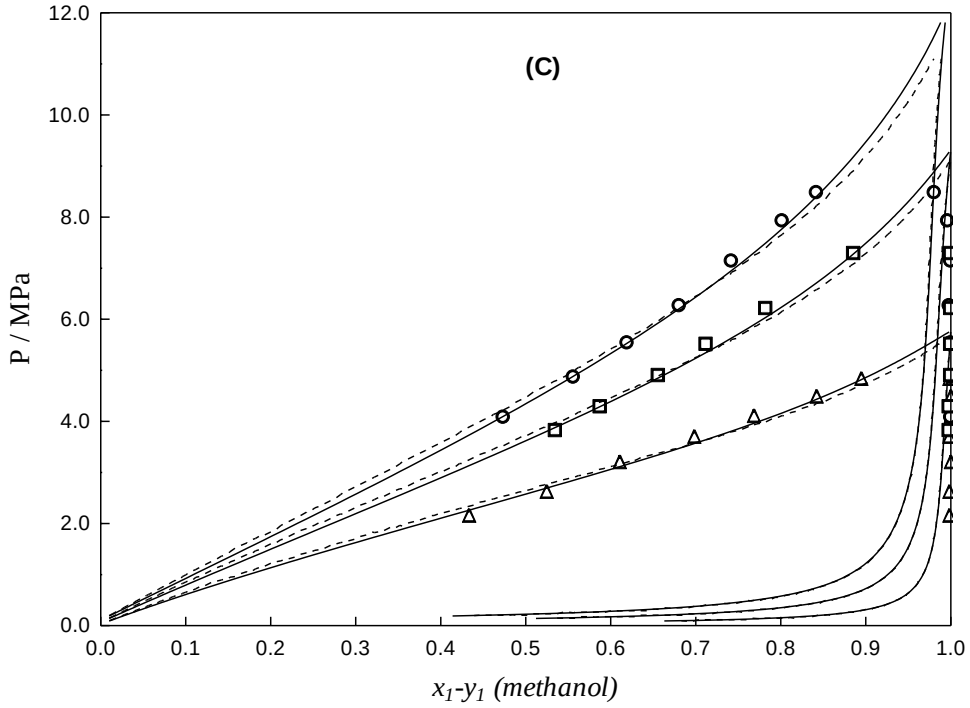

(B)
T / K
640
600
560
520
480
440
400
360
320
280
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
~ 92.0 kPa
~ 23.9 kPa
x1 (ethanol)

Figure 9


(A)
P / MPa
x_1-y_1 (ethanol)
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0


(B)
P / MPa
x_1-y_1 (ethanol)
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0



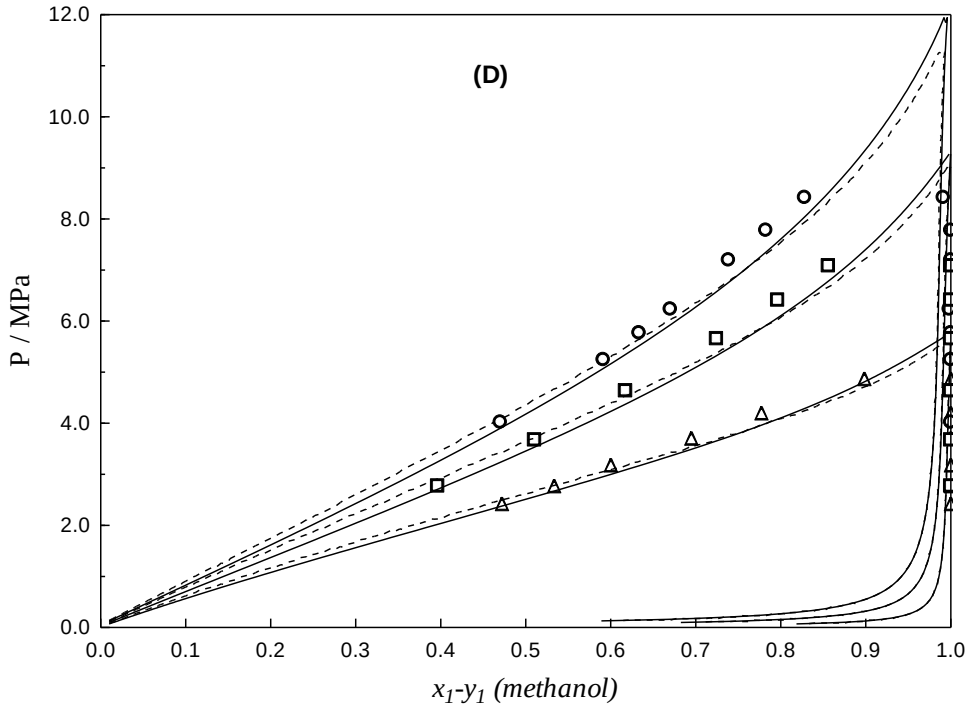


Figure 10