

Core-softened water-alcohol mixtures: the solute-size effects

Electronic Supplementary material

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1 Isobars with Temperature of Maximum Density (TMD)

1.1 Pure CSW potential

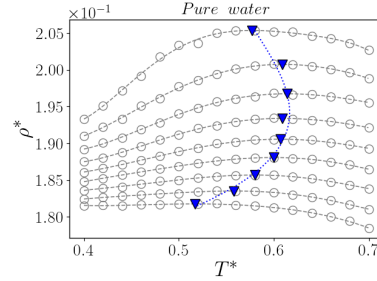


Figure 1: Isobars with temperature of maximum density (TMD) for pure CS water. From bottom to top: $P^* = 0.02, 0.03, 0.04, \dots, 0.10$.

1.2 Methanol

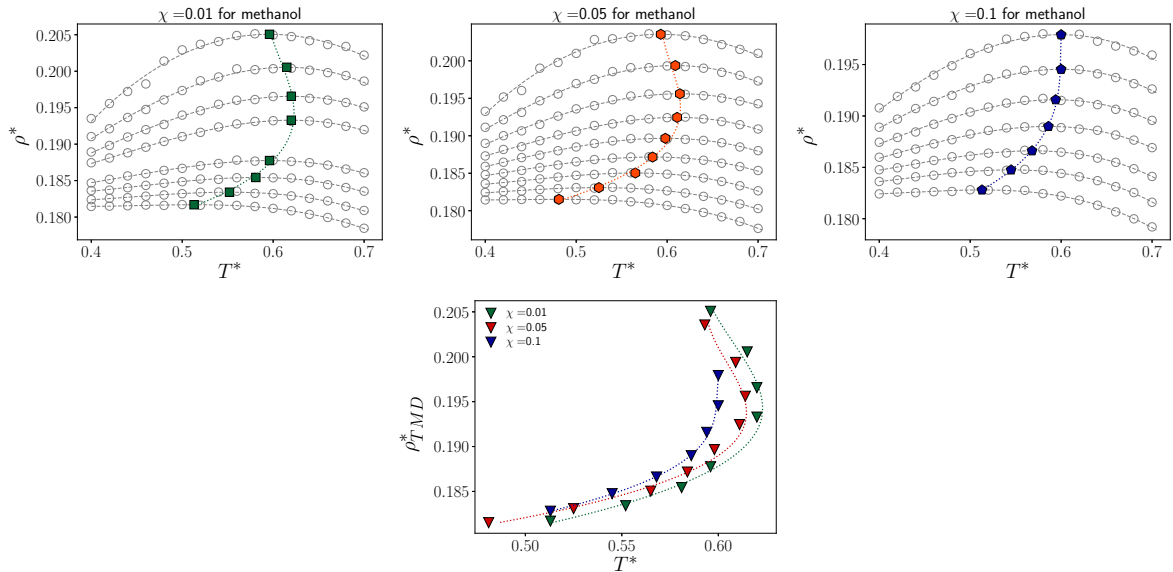


Figure 2: Isobars with temperature of maximum density (TMD) for all concentrations analyzed in methanol aqueous solutions. For two first concentrations ($\chi = 0.01$ and $\chi = 0.05$), and from bottom to top: $P^* = 0.02, 0.03, 0.04, \dots, 0.10$. For last concentration ($\chi = 0.10$), we have $P^* = 0.03, 0.04, \dots, 0.09$.

1.3 Ethanol

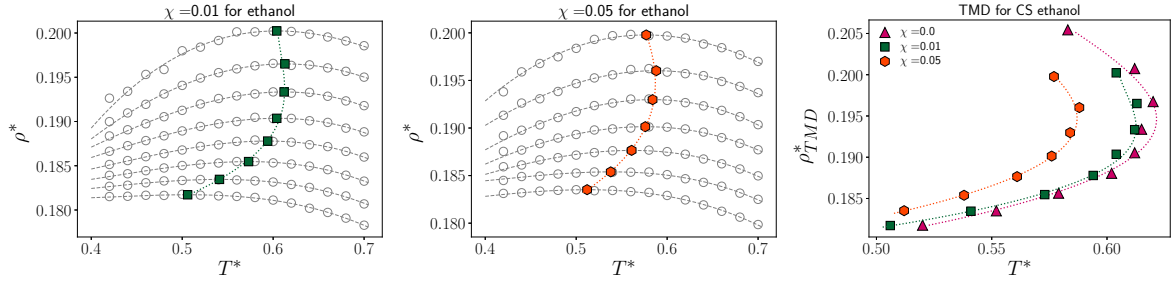


Figure 3: Isobars with temperature of maximum density (TMD) for all concentrations analyzed in ethanol aqueous solutions. For the first concentration ($\chi = 0.01$), and from bottom to top: $P^* = 0.02, 0.03, 0.04, \dots, 0.09$. For last concentration ($\chi = 0.05$), we have $P^* = 0.03, 0.04, \dots, 0.09$

1.4 Propanol

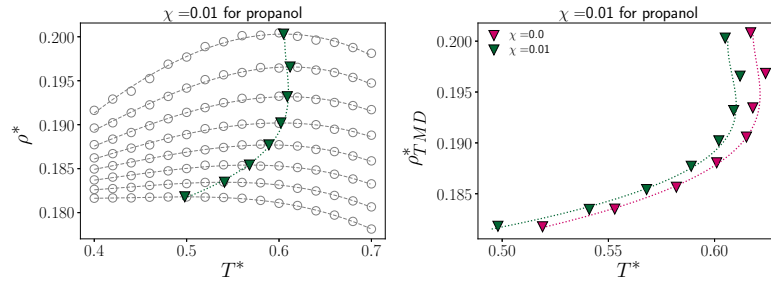


Figure 4: Isobars with temperature of maximum density (TMD) for all concentrations analyzed in propanol aqueous solutions. From bottom to top: $P^* = 0.02, 0.03, 0.04, \dots, 0.09$.

2 Isobars in Density-temperature plane for all solutions

2.1 Methanol

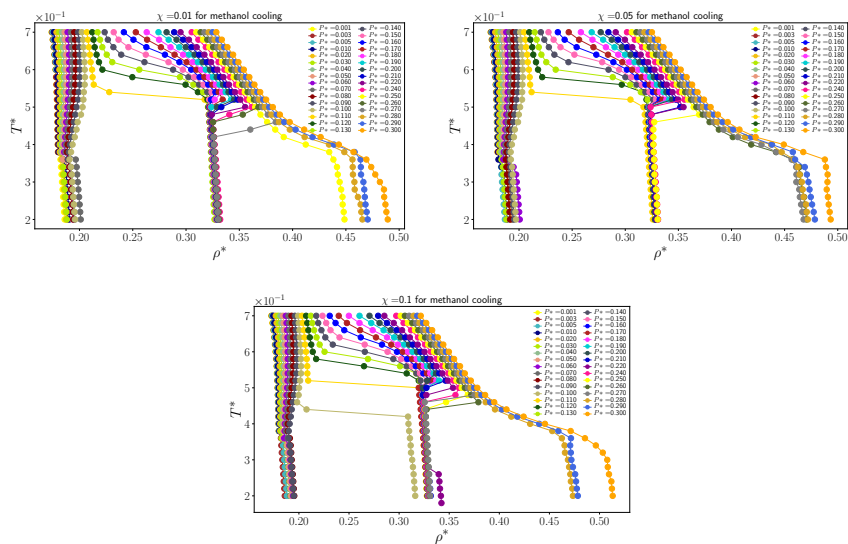


Figure 5: Isobars in aqueous solutions of methanol for all temperatures simulated in this work.

2.2 Ethanol

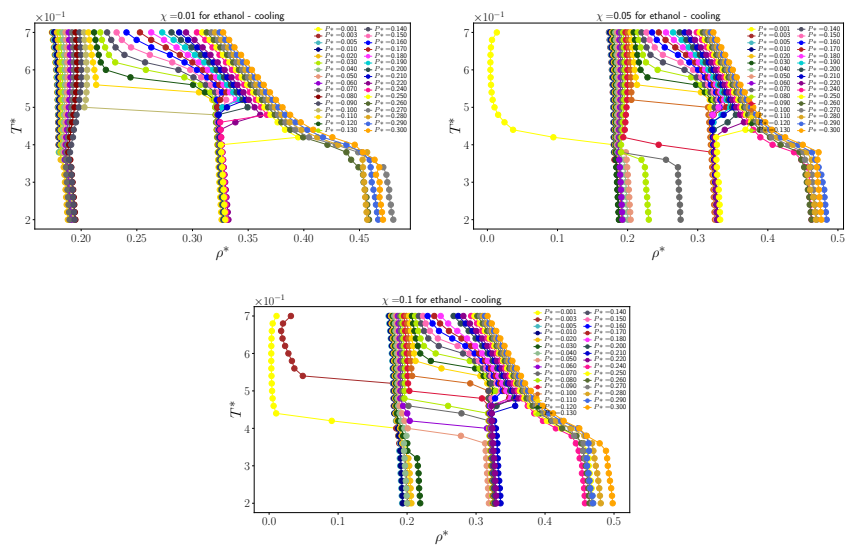


Figure 6: Isobars in aqueous solutions of ethanol for all temperatures simulated in this work.

2.3 Propanol

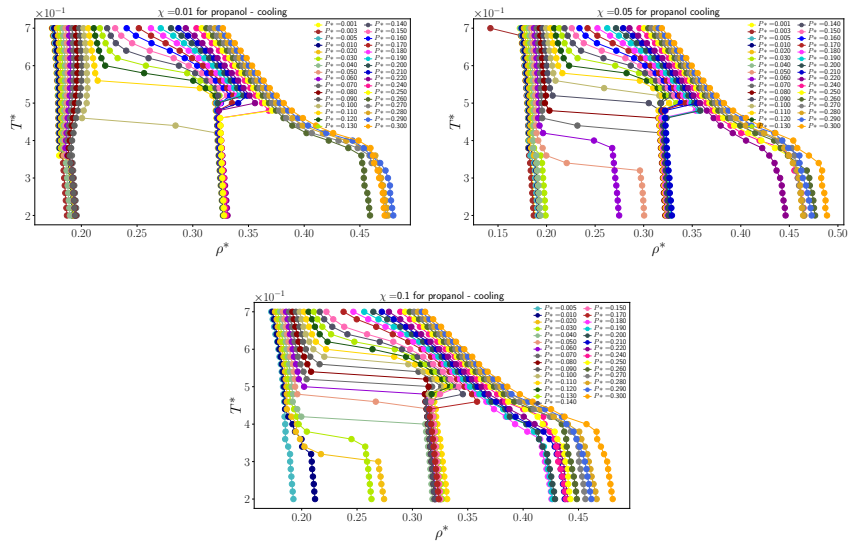


Figure 7: Isobars in aqueous solutions of propanol for all temperatures simulated in this work.

3 Peaks and discontinuities in Isothermal Compressibility

3.1 Pure CSW potential

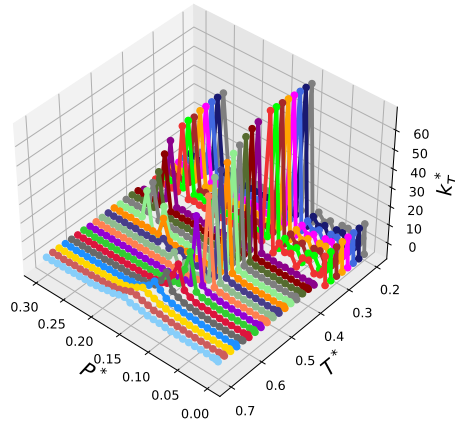


Figure 8: Peaks in κ_T for pure CSW potential ($x_1 = 0.00$).

3.2 Solutions of methanol, ethanol and 1-propanol

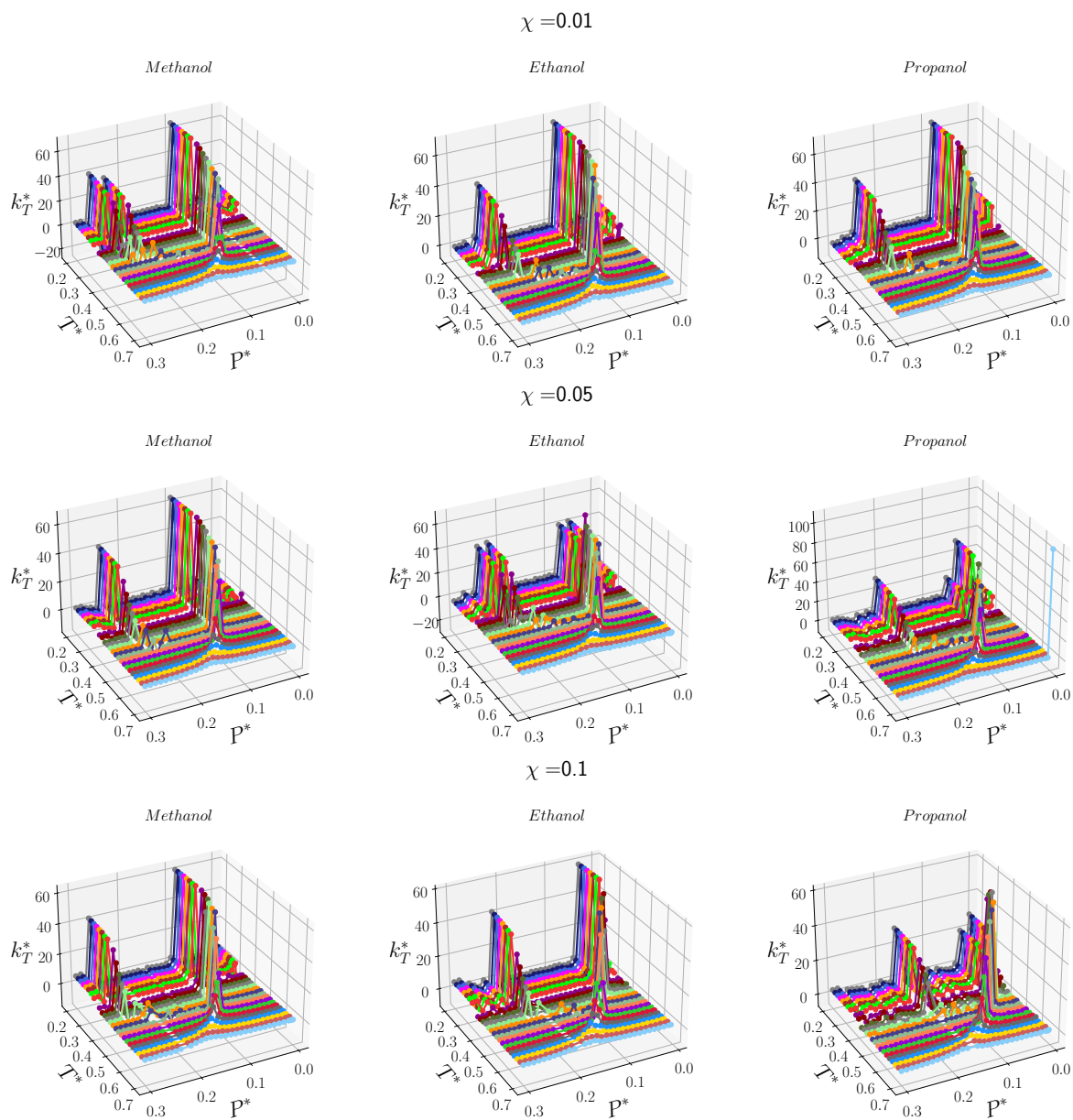


Figure 9: Peaks in κ_T for $x_1 = 0.01, 0.05$ and 0.1 .

4 Peaks and discontinuities in Specific heat at constant pressure

4.1 Pure CSW potential

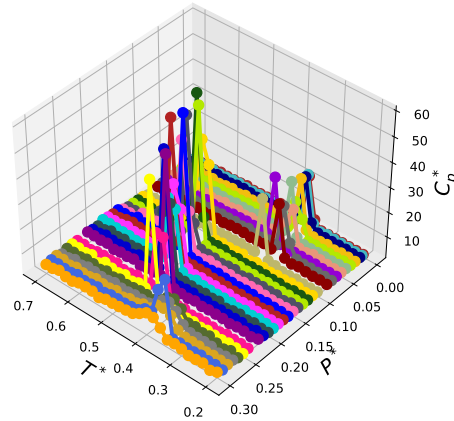


Figure 10: Peaks in $c_p(T)$ for pure CSW potential ($x_1 = 0.00$).

4.2 Solutions of methanol, ethanol and 1-propanol

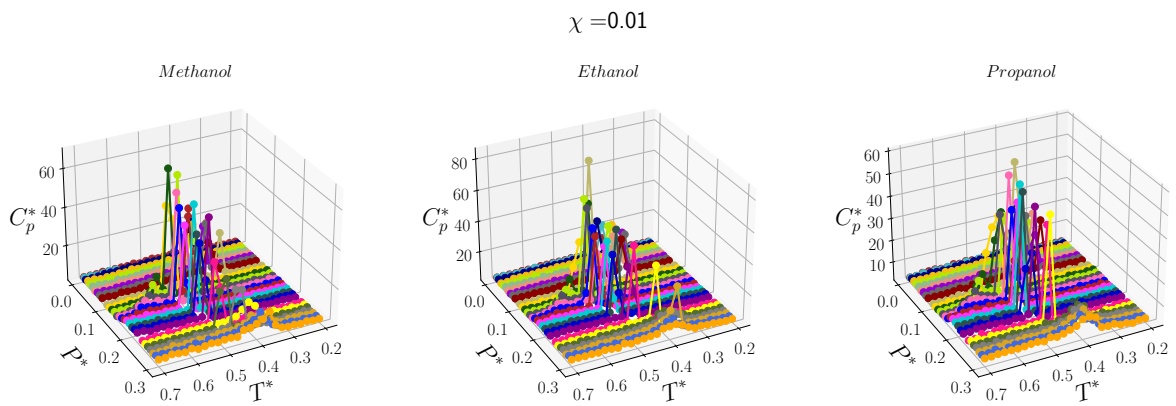


Figure 11: Peaks in $c_p(T)$ for $x_1 = 0.01$.

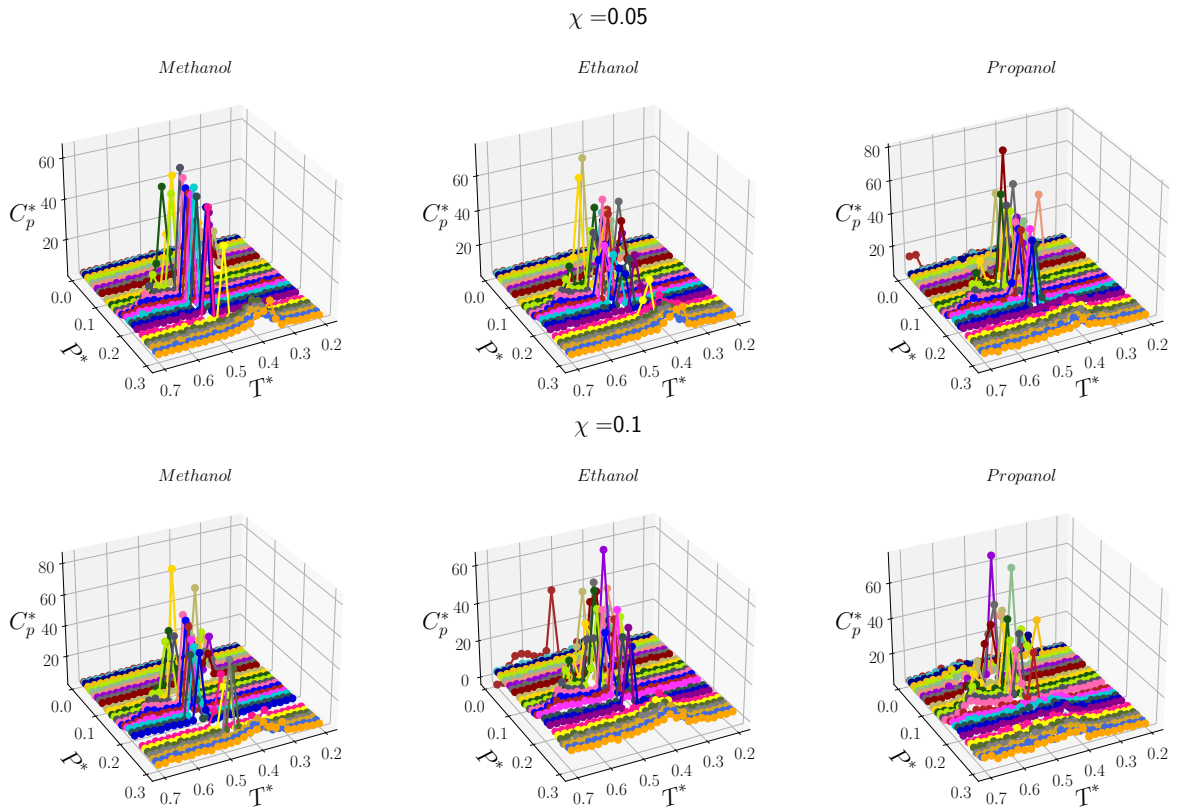


Figure 12: Peaks in $c_p(T)$ for $x_1 = 0.05$ and 0.1 .

5 Peaks and discontinuities in Isobaric compressibility coefficient of thermal expansion

5.1 Pure CSW potential

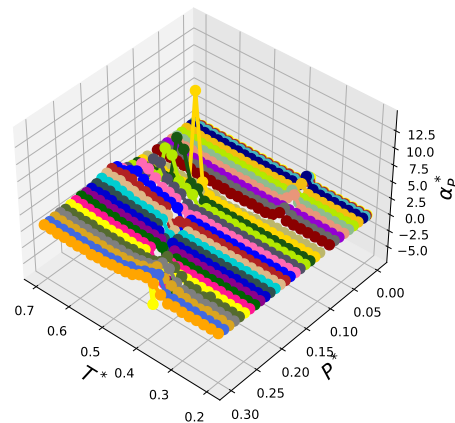


Figure 13: Peaks in $\alpha_p(T)$ for pure CSW potential ($x_1 = 0.00$).

5.2 Solutions of methanol, ethanol and 1-propanol

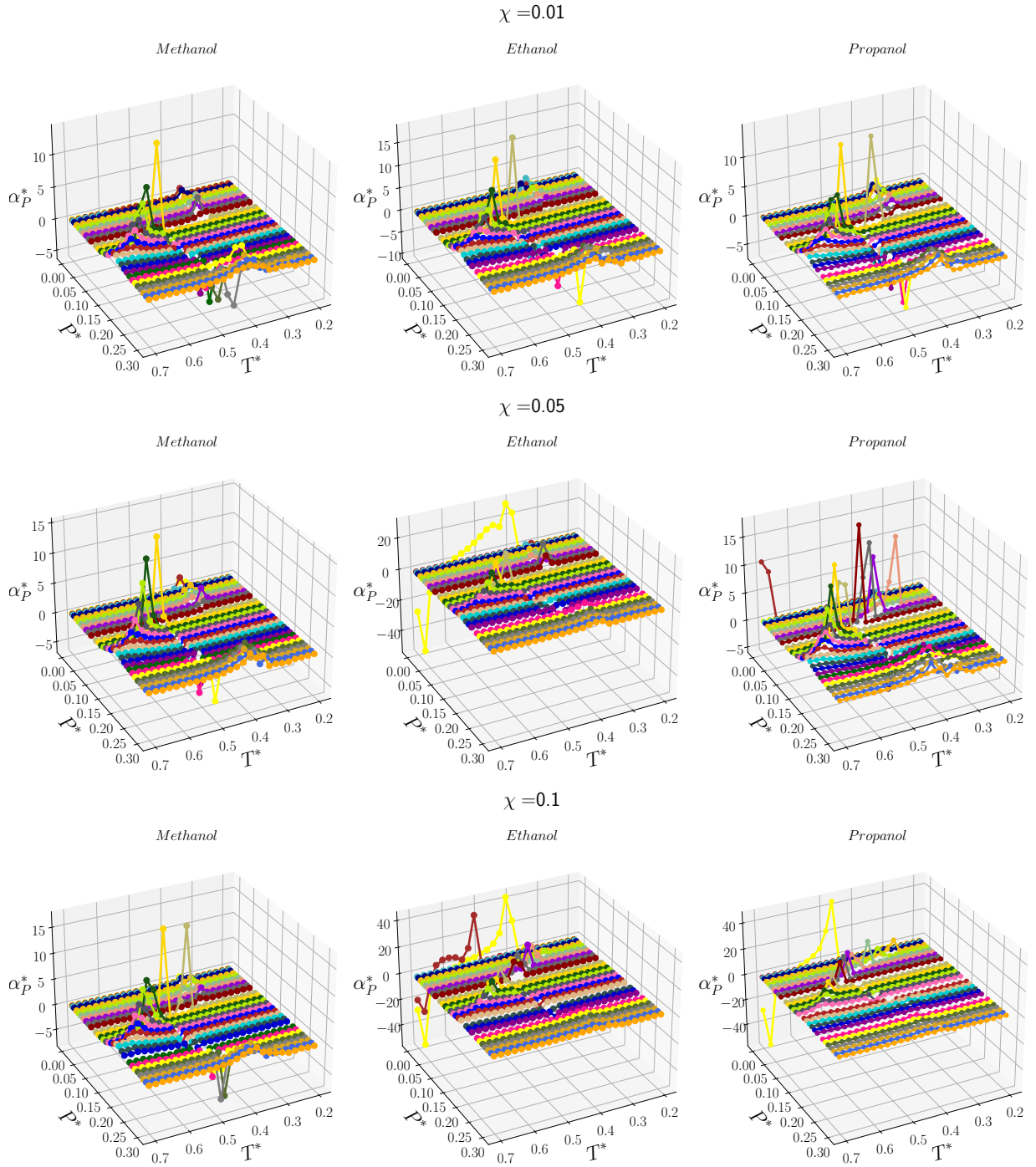


Figure 14: Peaks in $\alpha_P(T)$ for $x_1 = 0.01, 0.05$ and 0.1 .

6 Critical values

Pure CSW potential			
χ	P_c^*	T_c^*	ρ_c^*
0.00	0.125	0.590	0.2472
Methanol			
χ	P_c^*	T_c^*	ρ_c^*
0.01	0.120	0.590	0.250124
0.05	0.120	0.590	0.255124
0.10	0.130	0.590	0.259300
Ethanol			
χ	P_c^*	T_c^*	ρ_c^*
0.01	0.130	0.600	0.241481
0.05	0.130	0.600	0.242836
0.10	0.125	0.600	0.261500
Propanol			
χ	P_c^*	T_c^*	ρ_c^*
0.01	0.120	0.580	0.256308
0.05	0.110	0.590	0.249583
0.10	0.110	0.590	0.252400

Table 1: Critical values for pressure, temperature and density for all concentrations.

7 Structural order parameter for all solutions

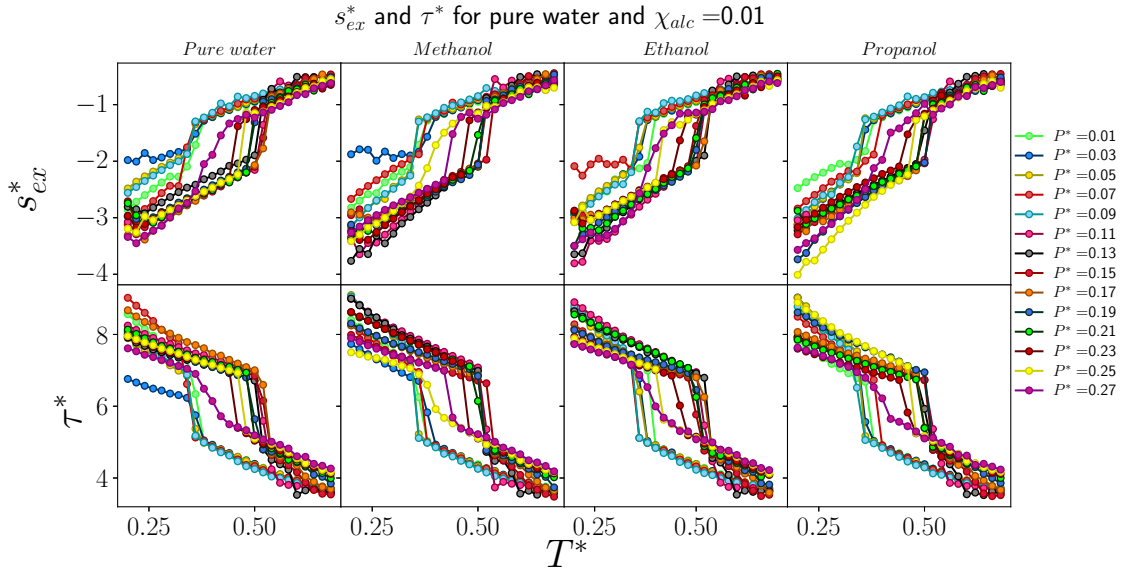


Figure 15: s_{ex}^* and τ^* behavior for ($\chi_{alc} = 0.01$).

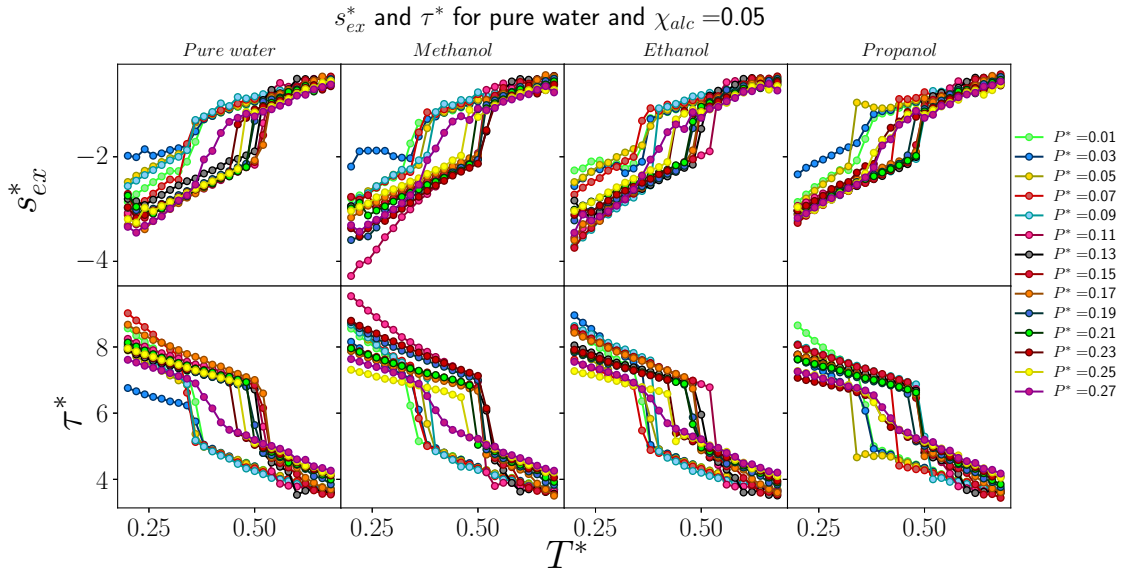


Figure 16: s_{ex}^* and τ^* behavior for ($\chi_{alc} = 0.05$).

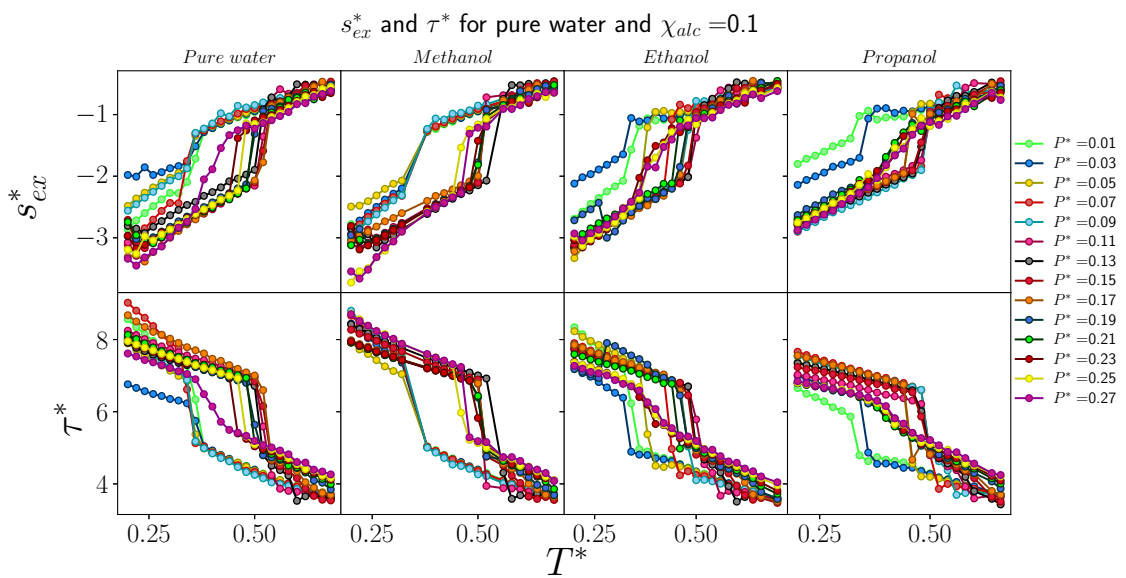


Figure 17: s_{ex}^* and τ^* behavior for ($\chi_{alc} = 0.10$).