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Supplementary material to

THERMODYNAMIC MODELING OF GAS SOLUBILITY IN IONIC LIQUIDS USING EQUATIONS OF STATE

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SUPPLEMENTARY A - CH_4, CO_2, and H_2S results
Supplementary A1. Parameters of the EoS

The section contains the parameters obtained for CH_4, CO_2, and H_2S from the SRK, CPA, and PC-SAFT EoS, which were taken from the literature, as shown in the following tables.

Table S1. Pure component parameters from SRK EoS [1].

Components	MM [g/mol]	T_c [K]	P_c [bar]	ω [-]
CH_4	16.04	190.56	45.99	0.0115478
CO_2	44.01	304.21	73.83	0.2236210
H_2S	34.08	373.30	89.63	0.0941677

Table S2. Pure component parameters from CPA EoS.

Components	MM [g/mol]	m_m [-]	T_{cm} [K]	P_{cm} [bar]	$\frac{\epsilon^{AB}}{R}$[K]	β^{AB} [-]	Associative schemes	Reference**
CH_4	16.04	0.4516	193.18	47.82			NA*	[2]
CO_2	44.01	0.7728	309.93	82.08				
H_2S	34.08	0.6389	313.35	77.97	454.87	0.2329	3B***	[3]

**NA: Non-associative. **The parameters b_{CPA}, a_0, c_1, ϵ^{AB} e β^{AB} were obtained and the parameters m_m, T_{cm}, P_{cm}, ϵ^{AB}/R e β^{AB} were calculated. ***3B: Associative type 3B.

Table S3. Pure component parameters from PC-SAFT EoS.

Components	MM [g/mol]	m [-]	σ [A]	$\frac{\varepsilon_{ij}}{k_b}$[K]	$\frac{\epsilon^{AB}}{k_b}$[K]	K^{AB} [-]	Associative schemes	Reference
CH_4	16.04	1.0000	3.7039	150.03			NA*	[4]
CO_2	44.01	2.0729	2.7852	16.21				
H_2S	34.08	1.6490	3.0550	229.84	536.6	0.001	2B**	[5]

*NA: Non-associative. **2B: Associative type 2B.

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Supplementary A2. Methane (CH_4) results

The first part of the development of the present work consisted of conducting tests with parameterizations indicated in the literature for the validation of the algorithm developed for estimating the parameters of ionic liquids. Thus, tests were performed with CH_4, CO_2, and H_2S. The following figures show the results obtained for the EoS CPA and PC-SAFT CH_4, CO_2, and H_2S. In summary, the algorithm proved to be able to be applied to ionic liquids. In addition, it is worth noting that the parameterizations applied to EoS for CH_4, CO_2, and H_2S were obtained from the literature.

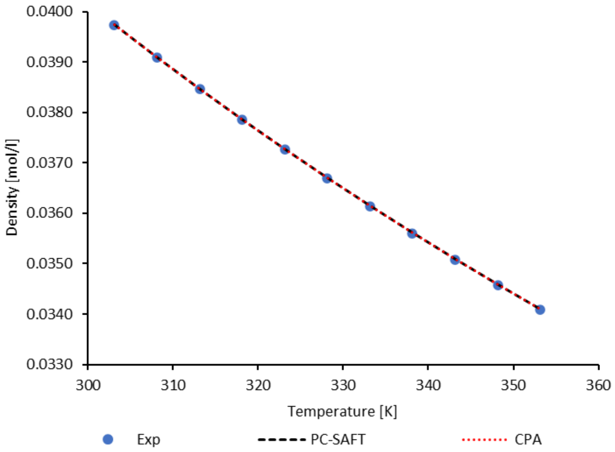

Figure S1. Density vs temperature data for CH_4 calculated by CPA and PC-SAFT EoS. Experimental data from NIST [6].

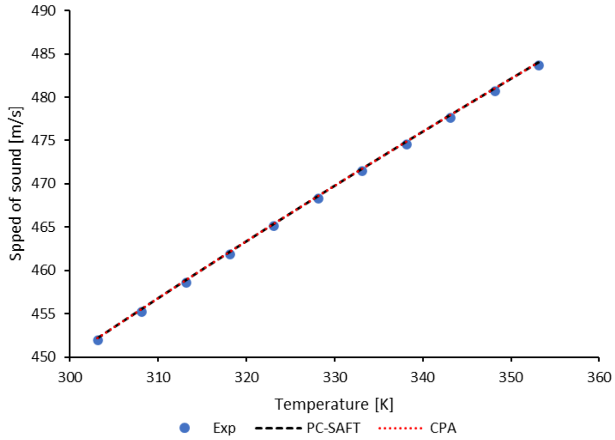

Figure S2. Speed of sound vs temperature data for CH_4 calculated by CPA and PC-SAFT EoS. Experimental data from NIST [6].

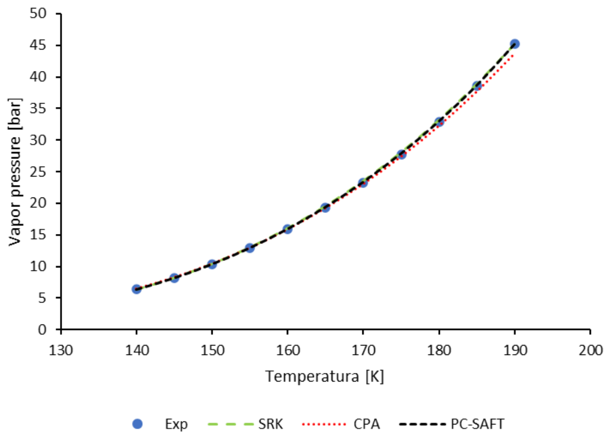

Figure S3. Vapor pressure vs temperature data for CH_4 calculated by SRK, CPA, and PC-SAFT EoS. Experimental data from NIST [6].

Supplementary A3. Carbon Dioxide (CO_2) results

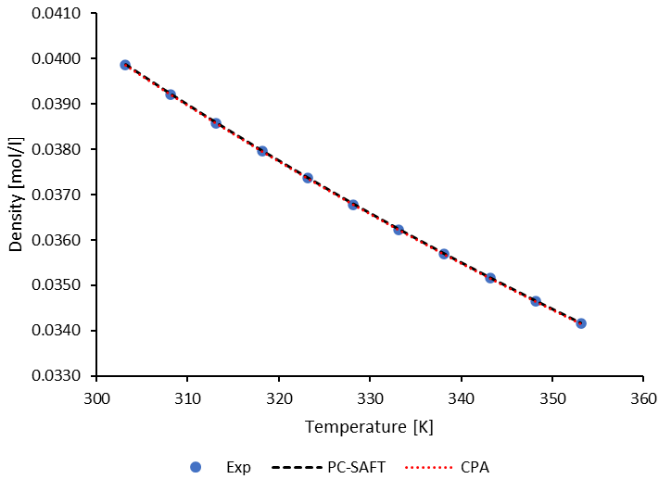

Figure S4. Density vs temperature data for CO_2 calculated by CPA and PC-SAFT EoS. Experimental data from NIST [6].

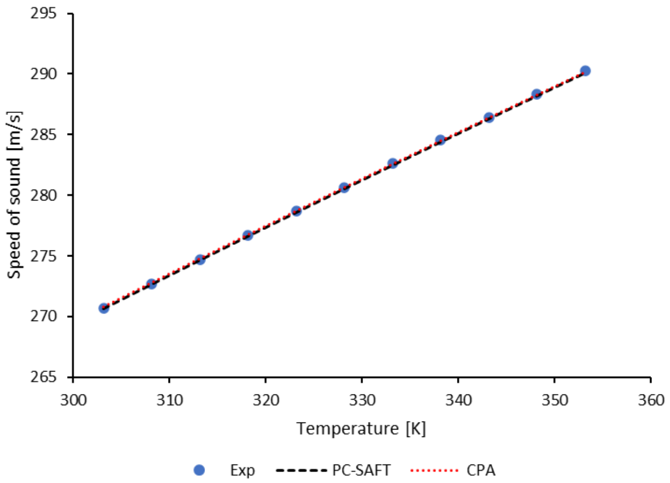

Figure S5. Speed of sound vs temperature data for CO_2 calculated by CPA and PC-SAFT EoS. Experimental data from NIST [6].

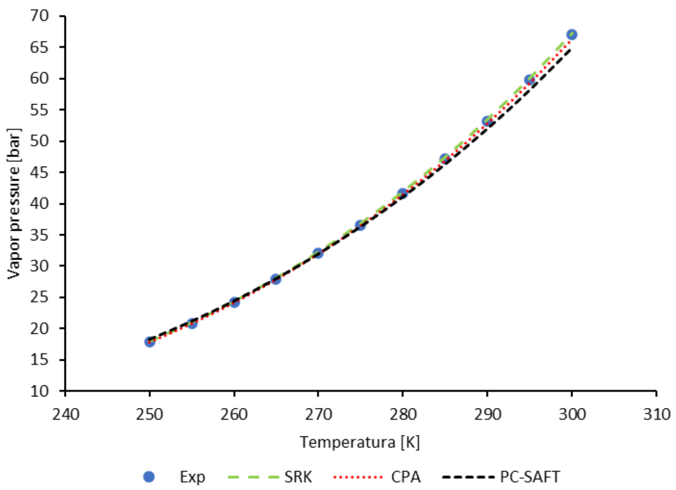

Figure S6. Vapor pressure vs temperature data for CO_2 calculated by SRK, CPA, and PC-SAFT EoS. Experimental data from NIST [6].

Supplementary A4. Hydrogen Sulfide (H_2S) results

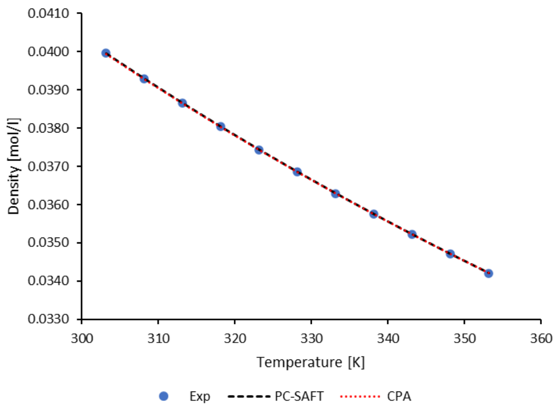

Figure S7. Density vs temperature data for H_2S calculated by CPA and PC-SAFT EoS. Experimental data from NIST [6].

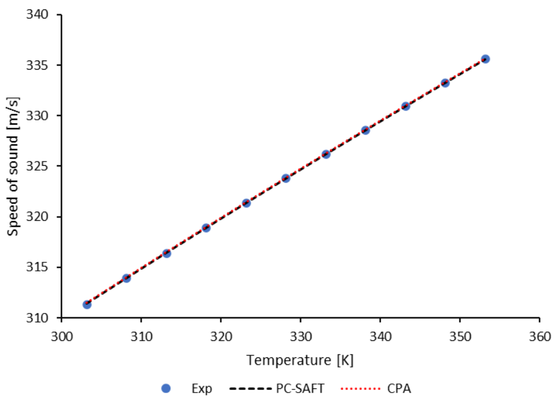

Figure S8. Density vs temperature data for H_2S calculated by CPA and PC-SAFT EoS. Experimental data from NIST [6].

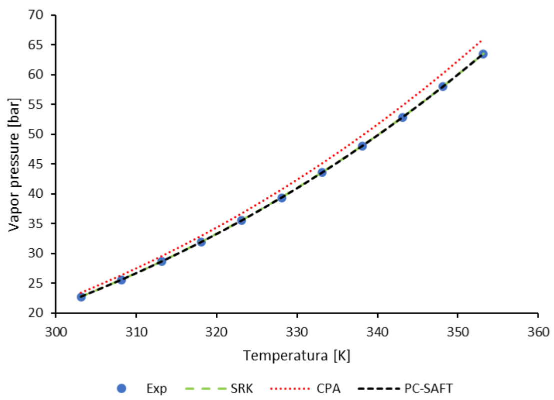

Figure S9. Vapor pressure vs temperature data for H_2S calculated by SRK, CPA, and PC-SAFT EoS. Experimental data from NIST [6].

SUPPLEMENTARY B – Calculation memory from SRK EoS

This section presents the equations used to solve the SRK model.

Supplementary B1. Helmholtz free energy

The physical contribution of the Helmholtz energy is given by Equation (S-B1).

$$\tilde{a}^{fis} = -\ln(1-b\rho) - q(T)/(\rho) \tag{S-B1}$$

where:

$$q(T) = \frac{a_0\ \alpha(T)}{b\ R\ T} \tag{S-B2}$$

$$I(\rho) = \frac{1}{\sigma - \varepsilon}\ln\left(\frac{1+\sigma\ b\ \rho}{1+\varepsilon\ b\ \rho}\right) \tag{S-B3}$$

$$\alpha(T) = \left(1 + c_1\ \left(1 - \sqrt{T_R}\right)\right)^2 \tag{S-B4}$$

It is important to highlight that T and ρ are independent variables and the terms a_0 and b are specific to each component. In addition, σ and ε are specific parameters of the equations of state, where they were obtained from Smith *et al.* [7].

Supplementary B2. Compressibility factor (Z)

The calculation of pressure and fugacity coefficient is given by:

$$P = Z^{fis}\rho\ R\ T \tag{S-B5}$$

$$\ln(\varphi) = \tilde{a}^{res} + Z^{fis} - 1 - \ln\left(Z^{fis}\right) \tag{S-B6}$$

where:

$$Z^{fis} = \frac{1}{1 - b\ \rho} - \frac{q(T)\ b\ \rho}{(1+\sigma\ b\ \rho)(1+\varepsilon\ b\ \rho)} \tag{S-B7}$$

Supplementary B3. Derivative from the compressibility factor (Z) with respect to density (ρ)

$$\rho\frac{dZ^{fis}}{d\rho} = \frac{b\ \rho}{(1-b\ \rho)^2} - \frac{q(T) b\ \rho\ \left(1-\varepsilon\ \sigma\ b^2\ \rho^2\right)}{\left[(1+\sigma\ b\ \rho)(1+\varepsilon\ b\ \rho)\right]^2} \tag{S-B8}$$

Supplementary B4. Derivative from the compressibility factor (Z) with respect to temperature (T)

$$T\frac{dZ^{fis}}{dT} = \frac{b\ \rho}{(1+\sigma\ b\ \rho)(1+\varepsilon\ b\ \rho)} q(T)(f_1 - 1) \tag{S-B9}$$

where:

$$f_1 = T\frac{d\ln\alpha}{dT} = -c_1\sqrt{\frac{T}{T_c\ \alpha(T)}} \tag{S-B10}$$

Supplementary B5. Speed of sound

$$\tilde{u}^{fis} = (f_1 - 1)\ q(T)\ I(\rho) \tag{S-B11}$$

where:

$$\tilde{u}^{res} = \tilde{u}^{fis} \tag{S-B12}$$

Supplementary B6. Heat capacity at constant volume

$$\tilde{C}_V^{fis} = \left[(f_1 - 1) f_2 + f_2\right] q(T) I(\rho) \tag{S-B13}$$

where:

$$f_2 = T\frac{d}{dT}\left(\frac{d\ln\alpha}{dT}\right) = T\frac{d^2\ln\alpha}{dT^2} = -\frac{c_1}{2\ \alpha(T)}\sqrt{T_R}\left(\sqrt{\alpha(T)} + c_1\ \sqrt{T_R}\right) \text{ and} \tag{S-B14}$$

$$\tilde{C}_V^{res} = \tilde{C}_V^{fis} \tag{S-B15}$$

SUPPLEMENTARY C – Calculation memory from CPA EoS

Supplementary C presents the equations used to solve the CPA model. It is worth noting that the contribution of the term physics is found in Supplementary B.

Supplementary C1. Helmholtz free energy

The residual Helmholtz energy for the CPA equation of state is the sum of the Helmholtz energy of the resulting physical part of the SRK (Supplementary B) plus the associative Helmholtz energy, as shown in EoS (S-C1).

$$\tilde{a}^{res} = \tilde{a}^{fis} + \tilde{a}^{assoc} \quad \text{(S-C1)}$$

The associative Helmholtz energy is given by Equation (S-C2).

$$\tilde{a}^{assoc} = \sum_{Ai} \left(\ln(X_{Ai}) + \frac{1 - X_{Ai}}{2} \right) \quad \text{(S-C2)}$$

Equation (S-C3) is a generalization of the equation proposed by Huang and Radosz (1990), which presents relationships between associative schemes 1A, 2B, 3B, and 4C.

$$X_{Ai} = \frac{-1 + \chi_3\, \rho\, \Delta^{Ai\ Bj} + \sqrt{\left(1 + \chi_4\, \rho\, \Delta^{Ai\ Bj}\right)^2 + \chi_2\, \rho\, \Delta^{Ai\ Bj}}}{\chi_1\, \rho\, \Delta^{Ai\ Bj}} \quad \text{(S-C3)}$$

Table S4. Associative schemes of constants.

Associative Schemes	χ_1	χ_2	χ_3	χ_4	Relation among X_i
1A	2	4	0	0	-
2B	2	4	0	0	$X_{A_i} = X_{B_i}$
3B	4	4	1	1	$X_{A_i} = X_{B_i}$; $X_{C_i} = 2.X_{A_i} - 1$
4C	4	8	0	0	$X_{A_i} = X_{B_i} = X_{C_i} = X_{D_i}$

where:

$$\Delta^{Ai\ Bj} = g(V_m)^{ref} \left[\exp\left(\frac{\varepsilon^{Ai\ Bj}}{RT} \right) - 1 \right] b_{ij}\ \beta^{Ai\ Bj} \quad \text{(S-C4)}$$

$$\eta = \frac{b}{4\ V_m} \quad \text{(S-C5)}$$

$$g(V_m)^{ref} = \frac{1}{1 - 1.9\ \eta} \quad \text{(S-C6)}$$

Supplementary C2. Compressibility factor (Z)

The calculation of the compressibility factor of the CPA equation of state is the sum of the compressibility factor of the physical part resulting from the SRK (Supplementary B) plus the associative compressibility factor (Equation S-C7).

$$Z = Z^{fis} + Z^{assoc} \quad \text{(S-C7)}$$

The calculation of pressure and fugacity coefficient is given by:

$$P = Z\ \rho\ R\ T \quad \text{(S-C8)}$$

$$\ln(\varphi) = \tilde{a}^{res} + Z - 1 - \ln(Z) \quad \text{(S-C9)}$$

$$Z^{assoc} = -(1 + d_1) \frac{1}{2} \sum_{Ai} (1 - X_{Ai}) \quad \text{(S-C10)}$$

where:

$$d_1 = \rho \frac{d \ln g}{d\rho} = \frac{1.9\ \eta}{1 - 1.9\ \eta} \quad \text{(S-C11)}$$

Supplementary C3. Derivative from the compressibility factor (Z) respect to density (ρ)

$$\rho \frac{dZ}{d\rho} = \rho \frac{dZ^{fis}}{d\rho} + \rho \frac{dZ^{assoc}}{d\rho} \quad \text{(S-C12)}$$

$$\rho \frac{dZ^{assoc}}{d\rho} = \frac{-1.9\ \eta}{(1 - 1.9\ \eta)^2} \frac{1}{2} \sum_{Ai} (1 - X_{Ai}) + (1 + d_1)\ \frac{1}{2} \sum p_{Ai} \quad \text{(S-C13)}$$

where:

$$p_{Ai} = \rho \frac{dX_{Ai}}{d\rho} = -\frac{\frac{1}{\chi_1}\left(\frac{\chi_2}{2} + \chi_3 + \chi_4 \right) - X_{Ai}}{1 + \rho\ \Delta^{Ai\ Bj} \left(X_{Ai}\ \chi_1 - \chi_3 \right)} (1 + d_1) \quad \text{(S-C14)}$$

Supplementary C4. Derivative from the compressibility factor (Z) with respect to (T)

$$T\frac{dZ}{dT}=T\frac{dZ^{fis}}{dT}+T\frac{dZ^{assoc}}{dT} \tag{S-C15}$$

$$T\frac{dZ^{assoc}}{dT}=\left(1+d_1\right)\ \frac{1}{2}\sum_{Ai}\left(t_{Ai}\right) \tag{S-C16}$$

where:

$$t_{Ai}=T\frac{dX_{Ai}}{dT}=q_1\left[\frac{o.5\chi_1+\left(\rho\ \Delta^{Ai\ Bj}\chi_4+1\right)\chi_4}{1-\left(\chi_4-X_{Ai}\ \chi_4\right)\rho\ \Delta^{Ai\ Bj}}+\chi_3-X_{Ai}\chi_1\right]\frac{1}{\chi_1} \tag{S-C17}$$

$$q_1=-\frac{\exp\left(\frac{\varepsilon^{Ai\ Bj}}{R\ T}\right)\ \frac{\varepsilon^{Ai\ Bj}}{R\ T}}{\exp\left(\frac{\varepsilon^{Ai\ Bj}}{R\ T}\right)-1} \tag{S-C18}$$

Supplementary C5. Speed of sound

$$\tilde{u}^{res}=\tilde{u}^{fis}+\tilde{u}^{assoc} \tag{S-C19}$$

The contribution of the associative speed of sound is given by Equation (S-C20).

$$\tilde{u}^{assoc}=\sum_{Ai}t_{Ai}\ g_{ai} \tag{S-C20}$$

where:

$$g_{ai}=\sum_{Ai}\left(\frac{1}{2}-\frac{1}{X_{Ai}}\right) \tag{S-C21}$$

Supplementary C6. Heat capacity at constant volume

$$\tilde{C}_V^{res}=\tilde{C}_V^{fis}+\tilde{C}_V^{assoc} \tag{S-C22}$$

The contribution of the associative heat capacity at constant volume is given by Equation (S-C23).

$$\tilde{C}_V^{assoc}=\sum_{Ai}L_{Ai}+\sum_{Ai}h_{Ai}g_{Ai} \tag{S-C23}$$

where:

$$L_{Ai}=\left(\frac{t_{Ai}}{X_{Ai}}\right)^2 \tag{S-C24}$$

$$h_{Ai}=\frac{d}{dT}\left(T^2\frac{dX_{Ai}}{dT}\right)=-\frac{v_{Ai}}{\Delta^{Ai\ Bj}}\left[t_{Ai}+G_1-G_2-\frac{1}{\chi_1}\ G_3\right]-\frac{1}{\chi_1}\ G_4\ G_5 \tag{S-C25}$$

$$v_{Ai}=T\ \frac{d\Delta^{Ai\ Bj}}{dT}=-b\ g\left(\rho\right)\beta^{Ai\ Bj}\exp\left(\frac{\varepsilon^{Ai\ Bj}}{R\ T}\right)\ \frac{\varepsilon^{Ai\ Bj}}{R\ T} \tag{S-C26}$$

$$G_1=\frac{\left[\rho\ \frac{v_1}{\chi_1}\ \left(X_{Ai}\chi_1-\chi_3\right)+\rho\ t_{ai}\ \Delta^{Ai\ Bj}\right]\left[0.5\ \chi_2+\left(\rho\ \Delta^{Ai\ Bj}\chi_4+1\right)\chi_4\right]}{\left[\rho\ \left(X_{Ai}\ \chi_1-\chi_3\right)\Delta^{Ai\ Bj}+1\right]^2} \tag{S-C27}$$

$$G_2=\frac{\rho\ \frac{v_{Ai}}{\chi_1}\ \left(\chi_4\right)^2}{\rho\ \left(X_{Ai}\ \chi_1-\chi_3\right)\Delta^{Ai\ Bj}+1} \tag{S-C28}$$

$$G_3=\left[\frac{0.5\ \chi_2+\left(\rho\ \Delta^{Ai\ Bj}\chi_4+1\right)\ \chi_4}{1-\left(\chi_3-X_{Ai}\ \chi_1\right)}+\chi_3-X_{Ai}\ \chi_1\right] \tag{S-C29}$$

$$G_4=\left[\frac{0.5\ \chi_2+\left(\rho\ \Delta^{Ai\ Bj}\chi_4+1\right)\ \chi_4}{\rho\ \left(X_{Ai}\ \chi_1-\chi_3\right)\Delta^{Ai\ Bj}+1}-X_{Ai}\ \chi_1+\chi_3\right] \tag{S-C30}$$

$$G_5 = \left[\frac{\frac{\varepsilon^{Ai\ Bj}}{R\ T} \exp\left(\frac{\varepsilon^{Ai\ Bj}}{R\ T}\right)\left(1 + \frac{\varepsilon^{Ai\ Bj}}{R\ T} - \exp\frac{\varepsilon^{Ai\ Bj}}{R\ T}\right)}{\left(\exp\left(\frac{\varepsilon^{Ai\ Bj}}{R\ T}\right) - 1\right)^2} \right] \tag{S-C31}$$

SUPPLEMENTARY D – Calculation memory from PC-SAFT EoS

Supplementary D presents the equations used to solve the PC-SAFT model.

$$\tilde{a}^{res} = \tilde{a}^{hs} + \tilde{a}^{chain} + \tilde{a}^{disp} + \tilde{a}^{assoc} \tag{S-D1}$$

Supplementary D1. Helmholtz free energy

The chain term is given by Equation S-D2:

$$\tilde{a}^{chain} = (1 - m_i)\ \ln\left(g_{ij}^{hs}(d_{ij})\right) \tag{S-D2}$$

where the radial distribution function $g_{ij}^{hs}(d_{ij})$:

$$g_{ij}^{hs}(d_{ij}) = \frac{1 - 0.5\ \eta}{(1-\eta)^3} \tag{S-D3}$$

The hard-sphere is given by Equation S-D4:

$$\tilde{a}^{hs} = m_i \frac{\eta\ (4 - 3\eta)}{(1-\eta)^2} \tag{S-D4}$$

where the coefficient η is:

$$\eta = \frac{\pi}{6} N_{av}\ \rho\ m_i \left(d_i(T)\right)^3 \tag{S-D5}$$

And the temperature-dependent segment diameter is:

$$d_i(T) = \delta_i \left[1 - 0.12\ \exp\left(-\frac{3\ \varepsilon_i}{k_B\ T}\right)\right] \tag{S-D6}$$

The dispersive term is given by Equation S-D7:

$$\tilde{a}^{disp} = \tilde{a}_A^{disp} + \tilde{a}_B^{disp} \tag{S-D7}$$

where:

$$\tilde{a}_A^{disp} = -2\ \pi\ \rho\ I_1\ m^2\ N_{av}\ \sigma_{ij}^3 \left(\frac{\varepsilon_{ij}}{k_B\ T}\right) \tag{S-D8}$$

$$\tilde{a}_B^{disp} = -\pi\ \rho\ \bar{m}\ C_1\ I_2\ m^2\ N_{av}\ \sigma_{ij}^3 \left(\frac{\varepsilon_{ij}}{k_B\ T}\right) \tag{S-D9}$$

$$C_1 = \left[1 + \bar{m}\frac{8\eta - 2\eta^2}{(1-\eta)^4} + \left(1 - \bar{m}\right)\frac{20\eta - 27\eta^2 + 12\eta^3 - 2\eta^4}{\left[(1-\eta)(2-\eta)\right]^2}\right]^{-1} \tag{S-D10}$$

$$I_1 = \sum_{i=0}^{6} a_i\left(\bar{m}\right)\eta^i \tag{S-D11}$$

$$I_2 = \sum_{i=0}^{6} b_i\left(\bar{m}\right)\eta^i \tag{S-D12}$$

$$a_i\left(\bar{m}\right) = a_{01} + \frac{\bar{m}-1}{\bar{m}} a_{1i} + \frac{\bar{m}-1}{\bar{m}}\ \frac{\bar{m}-2}{\bar{m}} a_{2i} \tag{S-D13}$$

$$b_i\left(\bar{m}\right) = b_{01} + \frac{\bar{m}-1}{\bar{m}} b_{1i} + \frac{\bar{m}-1}{\bar{m}}\ \frac{\bar{m}-2}{\bar{m}} b_{2i} \tag{S-D14}$$

The associative term is given by Equation S-C2, as for the CPA EoS and the associative term X_{A_i} is given by Equation (S-C3), however, in PC-SAFT case the $\Delta^{A_iB_j}$ is written as:

$$\Delta^{Ai\ Bj} = N_{av}\ \sigma_{ij}^3\ g_{ij}^{hs}(d_{ij})\left[\exp\left(\frac{\varepsilon^{Ai\ Bj}}{k_B\ T}\right) - 1\right]\kappa^{Ai\ Bj} \tag{S-D15}$$

Supplementary D2. Compressibility factor (Z):

$$Z = Z^{hs} + Z^{chain} + Z^{disp} + Z^{assoc} \tag{S-D16}$$

The hard-sphere is given by Equation S-D17:

$$Z^{hs} = 1 + m\frac{2\eta(2-\eta)}{(1-\eta)^3} \tag{S-D17}$$

The chain term is given by Equation S-D18:

$$Z^{chain} = -(m-1)\frac{\eta(5-2\eta)}{(1-\eta)(2-\eta)} \tag{S-D18}$$

The dispersive term is given by Equation S-D19:

$$Z^{disp} = Z_A^{disp} + Z_R^{disp} \tag{S-D19}$$

where:

$$Z_A^{disp} = -2\ \pi\ m^2\ N_{av}\ \sigma_{ij}^3\left(\frac{\varepsilon_{ij}}{kT}\right)\tilde{\rho}\ \frac{d}{d\eta}(\eta\ I_1) \tag{S-D20}$$

$$Z_B^{disp} = -\pi\ m^3\ N_{av}\ \sigma_{ij}^3\left(\frac{\varepsilon_{ij}}{kT}\right)^2\tilde{\rho}\ \left(C_1\frac{d}{d\eta}(\eta\ I_2)\right) + C_2\ \eta\ I_2 \tag{S-D21}$$

$$\frac{d}{d\eta}(\eta\ I_1) = \sum_{i=0}^{6} a_i(\overline{m})\ (i+1)\ \eta^i \tag{S-D22}$$

$$\frac{d}{d\eta}(\eta\ I_2) = \sum_{i=0}^{6} b_i(\overline{m})\ (i+1)\ \eta^i \tag{S-D23}$$

$$C_2 = -C_1\left[m\frac{(8+20\eta-4\eta^2)}{(1-\eta)^5} + (1-m)\frac{(40-48\eta+12\eta^2+2\eta^3)}{\left[(1-\eta)(2-\eta)\right]^3}\right] \tag{S-D24}$$

The associative term is given by Equation S-C8, in this case d_1 is:

$$d_1 = \rho\frac{d\ln g}{d\rho} = \frac{\eta}{2-\eta}\frac{5-2\eta}{1-\eta} \tag{S-E25}$$

Supplementary D3. Derivative from the compressibility factor (Z) respect to density (ρ)

$$\rho\frac{dZ}{d\rho} = \rho\frac{dZ^{hs}}{d\rho} + \rho\frac{dZ^{chain}}{d\rho} + \rho\frac{dZ^{disp}}{d\rho} + \rho\frac{dZ^{assoc}}{d\rho} \tag{S-E26}$$

The hard-sphere term is given by Equation S-D27:

$$\rho\frac{dZ^{hs}}{d\rho} = m\ \eta\frac{2(2+2\eta-\eta^2)}{(1-\eta)^4} \tag{S-D27}$$

The hard-sphere term is given by Equation S-D28:

$$\rho\frac{dZ^{chain}}{d\rho} = -(m-1)\ \eta\ \left[\frac{3}{(1-\eta)^2} - \frac{2}{(2-\eta)^2}\right] \tag{S-D28}$$

The dispersive term is given by Equation S-D29:

$$\rho\frac{dZ^{disp}}{d\rho} = A + B\ C \tag{S-D29}$$

where:

$$A = -2\ \pi\ \tilde{\rho}\ I_1\ m^2\ N_{av}\ \sigma_{ij}^3\left(\frac{\varepsilon_{ij}}{k_B\ T}\right)\ \frac{d}{d\eta}\left(\frac{\eta}{d\eta}\ \frac{I_1}{d\eta}\right) \tag{S-D30}$$

$$B = -\pi\ N_{av}\ \tilde{\rho}\ \sigma_{ij}^3\ m^3\left(\frac{\varepsilon_{ij}}{k_B\ T}\right)^2 \tag{S-D31}$$

$$C = 2\ \eta\ C_2\ \frac{d}{d\eta}(\eta\ I_2) + C_1\ \frac{d}{d\eta}\left(\frac{\eta}{d\eta}\ \frac{I_2}{d\eta}\right) + \eta\ I_2\ C_3 \tag{S-D32}$$

$$C_3 = C_2 + \frac{2\eta C_2{}^2}{C_1} - C_1^2\left[m\frac{12\eta(5+6\eta-\eta^2)}{(1-\eta)^6} + (m-1)\frac{6\eta(\eta^4+8\eta^3-48\eta^2+80\eta-44)}{(\eta^2-3\eta+2)^4}\right] \tag{S-D33}$$

$$\frac{d}{d\eta}\left(\frac{\eta}{d\eta}\ \frac{I_1}{d\eta}\right) = \sum_{i=0}^{6} a_i(\overline{m})(i+1)^2\ \eta^i \tag{S-D34}$$

$$\frac{d}{d\eta}\left(\frac{\eta}{d\eta}\ \frac{I_2}{d\eta}\right) = \sum_{i=0}^{6} b_i(\overline{m})(i+1)^2\ \eta^i \tag{S-D35}$$

The associative term is given by Equation S-D36:

$$\rho \frac{dZ^{assoc}}{d\rho} = N_1 \frac{1}{2}\sum_{Ai}(1-X_{Ai}) + (1+d_1)\frac{1}{2}\sum_{Ai} p_{Ai} \tag{S-D36}$$

where:

$$N_1 = \left[\frac{2\eta}{(2-\eta)^2} - \frac{3\eta}{(1-\eta)^2}\right] \tag{S-D37}$$

The parameter d_1 was obtained from Equation (S-D25), η from Equation (S-D5), and p_{A_i} from Equation (S-C14).

Supplementary D4. Derivative from the compressibility factor (Z) with respect to temperature (T)

$$T\frac{dZ}{dT} = T\frac{dZ^{hd}}{dT} + T\frac{dZ^{chain}}{dT} + T\frac{dZ^{disp}}{dT} + T\frac{dZ^{assoc}}{dT} \tag{S-D38}$$

The hard-sphere term is given by Equation S-D39:

$$T\frac{dZ^{hs}}{dT} = -\rho\frac{dZ^{hs}}{dT}F_1 \tag{S-D39}$$

where:

$$F_1 = \sigma_i \frac{1.08\ \exp\left(-\dfrac{3\ \varepsilon_i}{k_B\ T}\right)\dfrac{3\ \varepsilon_i}{k_B\ T}}{d_i(T)} \tag{S-D40}$$

The chain term is given by Equation S-D41:

$$T\frac{dZ^{chain}}{dT} = -\rho\ \frac{dZ^{chain}}{dT}F_1 \tag{S-D41}$$

The dispersive term is given by Equation S-D42:

$$T\frac{dZ^{disp}}{dT} = -\tilde{a}_A^{disp}\left[\frac{d}{d\eta}(\eta\ I_1) + F_1\left(\frac{d}{d\eta}\left(\frac{\eta}{d\eta}\frac{I_1}{d\eta}\right) - \frac{d}{d\eta}(\eta\ I_1)\right)\right] + F_2\left[F_3 + F_1(F_4 + F_5)\right] \tag{S-D42}$$

where:

$$F_2 = \pi\ m^3\ \rho\ N_{av}\ \sigma^3\left(\frac{\varepsilon_i}{k_B\ T}\right)^2 \tag{S-D43}$$

$$F_3 = 2\left(C_1\frac{d}{d\eta}(\eta\ I_2) + C_2\ \eta\ I_2\right) \tag{S-D44}$$

$$F_4 = 2\ C_2\ \eta\frac{d}{d\eta}(\eta\ I_2) + C_1\left(\frac{d}{d\eta}\left(\frac{\eta}{d\eta}\frac{I_2}{d\eta}\right) - \frac{d}{d\eta}(\eta\ I_2)\right) \tag{S-D45}$$

$$F_5 = \eta\ I_2(C_3 - C_2) \tag{S-D46}$$

The associative term is given by Equation S-D47:

$$T\frac{dZ^{assoc}}{dT} = (1+d_1)\ \frac{1}{2}\ \sum_{Ai}(t_{Ai}) - N_1\ F_1\ \frac{1}{2}\ \sum_{Ai}(1-X_{Ai}) \tag{S-D47}$$

where:

$$t_{Ai} = T\frac{dX_{Ai}}{dT} = \left[F_1\ (1+d_1) - N_2\right]N_3 \tag{S-D48}$$

$$N_2 = \frac{\exp\left(\dfrac{\varepsilon^{Ai\ Bj}\beta^{Ai\ Bj}}{k_B\ T}\right)\dfrac{\varepsilon^{Ai\ Bj}\beta^{Ai\ Bj}}{k_B\ T}}{\exp\left(\dfrac{\varepsilon^{Ai\ Bj}\beta^{Ai\ Bj}}{k_B\ T}\right) - 1} \tag{S-D49}$$

$$N_3 = \frac{1}{\chi_1}\left[\frac{0.5\ \chi_2 + (\rho\ \Delta\ \chi_4 + 1)\chi_4}{1 - (\chi_3 - X_{Ai}\ \chi_1)\rho\ \Delta} + \chi_3 - X_{Ai}\ \chi_1\right] \tag{S-D50}$$

Supplementary D5. Speed of sound

$$\tilde{u}^{res} = \tilde{u}^{hs} + \tilde{u}^{chain} + \tilde{u}^{disp} + \tilde{u}^{assoc} \tag{S-D51}$$

The hard-sphere is given by Equation S-D52:

$$\tilde{u}^{hs} = F_1\ (Z^{hs} - 1) \tag{S-D52}$$

The chain term is given by Equation S-D53:

$$\tilde{u}^{chain} = F_1\ Z^{chain} \tag{S-D53}$$

The dispersive term is given by Equation S-D54:

$$\tilde{u}^{disp} = \tilde{a}_A^{disp}\left[F_1\, F_6 + 1\right] + \tilde{a}_B^{disp}\left(F_1\, F_7 + 2\right) \tag{S-D54}$$

where:

$$F_6 = \frac{\frac{d}{d\eta}\left(\eta\ I_1\right)}{I_1} - 1 \tag{S-D55}$$

$$F_7 = \frac{C_2\ \eta}{C_1} + \frac{\frac{d}{d\eta}\left(\eta\ I_2\right)}{I_2} - 1 \tag{S-D56}$$

The associative term is given by Equation S-D57:

$$\tilde{u}^{assoc} = \sum_{Ai} t_{Ai}\ J_{Ai} \tag{S-D57}$$

where:

$$J_{Ai} = \frac{1}{2} - \frac{1}{X_{Ai}} \tag{S-D58}$$

Supplementary D6. Heat capacity at volume constant

$$\tilde{C}_V^{res} = \tilde{C}_V^{hs} + \tilde{C}_V^{chain} + \tilde{C}_V^{disp} + \tilde{C}_V^{assoc} \tag{S-D59}$$

The hard-sphere term is given by Equation S-D60:

$$\tilde{C}_V^{hs} = \left(Z^{hs} - 1\right)F_8 + F_1\ T\,\frac{dZ^{hs}}{dT} \tag{S-D60}$$

where:

$$F_8 = \frac{3.24\exp\left(-\frac{3\ \varepsilon_i}{k_B\ T}\right)\ \frac{3\ \varepsilon_i}{k_B\ T}}{\left[1 - 0.12\exp\left(-\frac{3\ \varepsilon_i}{k_B\ T}\right)\right]^2} \tag{S-D61}$$

The chain term is given by Equation S-D62:

$$\tilde{C}_V^{chain} = Z^{chain} F_8 + F_1\ T\,\frac{dZ^{chain}}{dT} \tag{S-D62}$$

The dispersive term is given by Equation S-D63:

$$\tilde{C}_V^{disp} = \tilde{C}_{V_1}^{disp} + \tilde{C}_{V_2}^{disp} \tag{S-D63}$$

where:

$$\tilde{C}_{V_1}^{disp} = -\tilde{a}_A^{disp}\ F_1\left(F_6\ F_{10} + F_9\ F_1\right) \tag{S-D64}$$

$$\tilde{C}_{V_2}^{disp} = -\tilde{a}_B^{disp}\ \left(F_1\ F_7 + 2\right)\left(F_1\ F_7 + 1\right) - F_1\ F_7\ F_{11} + F_1\ F_{12} \tag{S-D65}$$

$$F_9 = \frac{\frac{d}{d\eta}\left(\frac{\eta}{d\eta}\frac{I_1}{d\eta}\right)}{I_1} - 1 \tag{S-D66}$$

$$F_{10} = \frac{-0.24\exp\left(-\frac{3\ \varepsilon_i}{k_B\ T}\right)\ \left(9\frac{\varepsilon_i}{k_B\ T} + 1\right) + 2 - 3\frac{\varepsilon_i}{k_B\ T}}{d_i\left(T\right)} \tag{S-D67}$$

$$F_{11} = \sigma_i\,\frac{3\frac{\varepsilon_i}{k_B\ T} - \frac{\sigma_i}{d_i\left(T\right)}}{d_i\left(T\right)} \tag{S-D68}$$

$$F_{12} = \frac{C_2\ \eta}{C_1}\left(\frac{C_3}{C_2} - \frac{C_2\ \eta}{C_1}\right) + \frac{\frac{d}{d\eta}\left(\frac{\eta}{d\eta}\ \frac{I_2}{d\eta}\right)}{I_2} - \left(\frac{\frac{d}{d\eta}\left(\eta\ I_2\right)}{I_2}\right)^2 \tag{S-D69}$$

The associative term is given by Equation S-D70:

$$\tilde{C}_V^{assoc} = \sum_{Ai} L_{Ai} + \sum_{Ai} h_{Ai}\ J_{Ai} \tag{S-D70}$$

Where is given by Equation S-C24 and:

$$h_{Ai} = \frac{d}{dT}\left(T^2\,\frac{dX_{Ai}}{dT}\right) = -\frac{v_{Ai}}{\Delta^{Ai\ Bj}}\left[t_{Ai} + G_1 - G_2 - \frac{1}{\chi_1}G_3\right] - \frac{1}{\chi_1}G_4\ G_5 + G_6 \tag{S-D71}$$

$$v_{Ai} = T\frac{d\Delta^{Ai\ Bj}}{dT} = \Delta^{Ai\ Bj}\left[F_1\ (1+d_1) - N_2\right] \quad \text{(S-D72)}$$

The terms G_1 to G_5 are given from equation (S-C27) to (S-C31) and

$$G_6 = F_1\left[\left(3\frac{\varepsilon_i}{k_B\ T} - 1\right)\ (1+d_1) + F_1\ N_1\right] + G_7 \quad \text{(S-D73)}$$

$$G_7 = \sigma_i^2\frac{0.388\left(\frac{\varepsilon_i}{k_B\ T}\right)^2 \exp\left(-6\frac{\varepsilon_i}{k_B\ T}\ (1+d_1)\right)}{\left(d\ (T)\right)^2} \quad \text{(S-D74)}$$

SUPPLEMENTARY E – Ionic liquids results

In Supplementary E are presented the estimated parameters for ionic liquids, constants of the C_p^{gi} equation, the absolute average relative deviations of the equations of state, and the corresponding curves for methane, acid gases, ionic liquids, and solubility between ILs and other mentioned components.

Time is a major factor for everyday applications, which is worth noting that the estimation time of the parameters of ionic liquids, in which [EMIM][TfO] presented an estimation duration of 9 min 28 s for SRK EoS and non-associative CPA.

On the other hand, the associative CPA presented an average time of 48 min (which showed differences with the use of the associative scheme and parameter) and the non-associative PC-SAFT presented a duration of 43 min 26 s, while the associative PC-SAFT had an average of 1 h 54 min.

Nevertheless, [OMIM][NTf_2] presented an estimation duration of 23min33s for the SRK EoS and non-associative CPA, the average duration of 1 h 56 min for the CPA (which showed differences with the associative scheme and in the associative parameter) and the non-associative PC-SAFT had a duration of 2 h 40 min, while for the associative PC-SAFT it had an average of 5h05min. Furthermore, the Swarm method used to estimate the parameters was applied five hundred iterations and one hundred particles for all cases analyzed. In conclusion, the estimation time of the parameters of the studied EoS was shorter for the SRK and longer for the PC-SAFT, given the complexity of the resolution of these models. It is also worth noting that the estimation time increased according to the amount of experimental data, which could be seen by analyzing the mean times between the ionic liquids [EMIM][TfO] and [OMIM][NTf_2] for the SRK, which were from 9 min 28 s and 23 min 33 s, respectively; associative CPA which were 48 min and 1 h 56 min, respectively; the non-associative PC-SAFT were 43min26s and 2 h 40 mins, respectively; and, finally, the associative PC-SAFT which lasted 1 h 54 min and 5 h 05 min. Thus, it is necessary to verify if the computational effort spent in estimating the parameters of the pure components favors the prediction of the solubilities of the components in ionic liquids.

For that, the algorithm for estimating the parameters of the equations of state was developed in the Visual Studio Code source code editor in Python programming language, using a computer with a 64-bit Windows 10 Home Single Language operating system, Intel processor ® Core™ i5-8250U @1.60GHz CPU, 20.0GB @2133MHz RAM, Intel® UHD Graphics 620 processor graphics, 120GB SSD with reading speed up to 500MB/s and exclusive 1TB WDC HDD for storage.

Supplementary E1. EoS parameters

Table S5. Parameters of the C_p^{gi} equation for the SRK and CPA EoS.

Components	C_{1i}	C_{2i}	C_{3i}	C_{4i}	C_{5i}	β^{AB}	Model
[EMIM][TfO]	1906.93	-3.00803	0.00243	-21816563	-334428		SRK*
	1812.39	-2.83041	0.00231	-20181062	-315543	1	(1A)
	746.07	-0.57261	0.00053	-2972734	-95732	1	(2B)
	746.07	-0.57261	0.00053	-2972734	-95732	0.1	(2B)
	746.07	-0.57261	0.00053	-2972734	-95732	0.001	(2B)
	746.07	-0.57261	0.00053	-2972734	-95732	0.00001	(2B)
	746.07	-0.57261	0.00053	-2972734	-95732	1	(3B)
	856.04	-0.78345	0.00068	-5707203	-128975	1	(4C)
[OMIM][NTf_2]	54380.38	-125.70758	0.11048	-728483247	-10291960		SRK*
	63033.30	-144.77432	0.12627	-861847080	-12051169	1	(1A)
	57646.83	-133.22209	0.11704	-777254751	-10953470	1	(2B)
	52323.73	-121.56937	0.10748	-695112161	-9873353	0.1	(2B)
	76296.58	-174.96182	0.15201	-1051597543	-14650452	0.001	(2B)
	60021.48	-137.94008	0.12045	-819419049	-11473963	0.00001	(2B)
	57646.83	-133.22209	0.11704	-777254751	-10953470	1	(3B)
	51619.99	-120.53575	0.10715	-681362527	-9724358	1	(4C)

*SRK: Soave-Redlich-Kwong is the same for non-associative CPA. $\left(C_p^{gi}, J\ mol^{-1}\ K^{-1}\right) = C_{1i} + C_{2i}\left(T,K\right) + C_{3i}\left(T,K\right)^2 - \frac{C_{4i}}{\left(T,K\right)^2} + \frac{C_{5i}}{\left(T,K\right)}$

Table S6. Parameters of the C_p^{gi} equation for the PC-SAFT EoS.

Components	C_{1i}	C_{2i}	C_{3i}	C_{4i}	C_{5i}	K^{AB}	Model
[EMIM][TfO]	-2062.10	5.41885	-0.00422	39509475	441814		NA*
	51.23	0.94879	-0.00065	5509111	209	1	(1A)
	442.24	0.19566	-0.00010	-1130439	-86513	1	(2B)
	442.24	0.19566	-0.00010	-1130439	-86513	0.1	(2B)
	442.24	0.19566	-0.00010	-1130439	-86513	0.001	(2B)
	442.24	0.19566	-0.00010	-1130439	-86513	0.00001	(2B)
	8718.79	-17.58111	0.01420	-133361977	-1796310	1	(3B)
	81.01	1.12612	-0.00095	4304740	-20470	1	(4C)
[OMIM][NTf$_2$]	59836.51	-138.07784	0.12146	-801838185	-11334897		NA*
	55897.85	-129.29266	0.11415	-742967569	-10550518	1	(1A)
	56780.91	-131.10416	0.11557	-757683454	-10739526	1	(2B)
	56780.91	-131.10416	0.11557	-757683454	-10739526	0.1	(2B)
	86561.74	-195.15190	0.16719	-1233765944	-16890129	0.001	(2B)
	53592.67	-123.27552	0.10831	-717995147	-10159673	0.00001	(2B)
	61452.95	-141.27142	0.12386	-831036297	-11695363	1	(3B)
	58500.50	-134.55250	0.11817	-786883440	-11112937	1	(4C)

* NA: Non-associative. $\left(C_p^{gi}, J\ mol^{-1}\ K^{-1}\right) = C_{1i} + C_{2i}\left(T,K\right) + C_{3i}\left(T,K\right)^2 - \frac{C_{4i}}{\left(T,K\right)^2} + \frac{C_{5i}}{\left(T,K\right)}$

Table S7. Estimated parameters of the ionic liquids from the RK-Aspen model.

Components	MM [g/mol]	T_c^*[K]	P_c^*[bar]	ω[-]	Estimation time
[EMIM][TfO]	260.23	1217.53	49.742	0.01164	9 min 28 s
[OMIM][NTf$_2$]	475.47	581.50	12.287	2.44405	23 min 33 s

Table S8. Estimated parameters of the ionic liquids from CPA EoS.

Components	β^{AB}** or K^{AB}***	Associative schemes	CPA Estimation time	PC-SAFT Estimation time
[EMIM][TfO]		NA*	9 min 28 s	43 min 26 s
	1	1A	46 min 17 s	1 h 55 min
	1	2B	49 min 15 s	1 h 49 min
	0.1	2B	48 min 12 s	1 h 53 min
	0.001	2B	50 min 04 s	1 h 58 min
	0.00001	2B	50 min 35 s	1 h 54 min
	1	3B	46 min 26 s	1 h 56 min
	1	4C	45 min 15 s	1 h 51 min
[OMIM][NTf$_2$]		NA*	23 min 33 s	2 h 40 min
	1	1A	1 h 54 min	5 h 08 min
	1	2B	1 h 55 min	5 h 03 min
	0.1	2B	1 h 53 min	5 h 05 min
	0.001	2B	2 h 02 min	5 h 04 min
	0.00001	2B	1 h 58 min	5 h 02 min
	1	3B	1 h 56 min	5 h 09 min
	1	4C	1 h 57 min	5 h 03 min

* NA: Non-associative. ** β^{AB}: for CPA EoS. ***K^{AB}: for PC-SAFT EoS.

Table S9. Regressed parameters in [SI] for [EMIM][TfO] (i) for CH_4, CO_2, and H_2S (j) with the RK-Aspen model.

Parameters	k_{aij}^0	$k_{aij}^1\left[\frac{1}{T}\right]$	k_{bij}^0	k_{bij}^1
[EMIM][TfO] / CH_4				
2p	0.05696	0	0.00570	0
4p	-0.00168	0.11650	-0.06598	0.20602
[EMIM][TfO] / CO_2				
Parameters	k_{aij}^0	$k_{aij}^1\left[\frac{1}{T}\right]$	k_{bij}^0	k_{bij}^1
2p	0.09333	0	0.03200	0
4p	0.13593	-0.19652	-0.01032	0.10532
[EMIM][TfO] / H_2S				
Parameters	k_{aij}^0	$k_{aij}^1\left[\frac{1}{T}\right]$	k_{bij}^0	k_{bij}^1
2p	0.03711	0	0.03236	0
4p	0.11858	-0.25830	0.07277	-0.12887

$$a_{ij} = \sqrt{a_i a_j}\left(1 - k_{aij}^0 - k_{aij}^1 \frac{T}{1000}\right);\ b_{ij} = \frac{b_i + b_j}{2}\left(1 - k_{bij}^0 - k_{bij}^1 \frac{T}{1000}\right).$$

Table S10. Regressed parameters in [SI] for [OMIM][NTf$_2$] (i) for CO_2 and H_2S (j) with the RK-Aspen model.

		[OMIM][NTf$_2$] / CO_2		
Parameters	k_{aij}^0	$k_{aij}^1 \left[\frac{1}{T}\right]$	k_{bij}^0	k_{bij}^1
2p	-0.05199	0	0.02328	0
4p	0.48683	-1.68080	0.03427	-0.04782
		[OMIM][NTf$_2$] / H_2S		
Parameters	k_{aij}^0	$k_{aij}^1 \left[\frac{1}{T}\right]$	k_{bij}^0	k_{bij}^1
2p	-0.04887	0	0.02357	0
4p	0.36222	-1.28246	0.00886	0.02947

$$a_{ij} = \sqrt{a_i a_j}\left(1 - k_{aij}^0 - k_{aij}^1 \frac{T}{1000}\right);\ b_{ij} = \frac{b_i + b_j}{2}\left(1 - k_{bij}^0 - k_{bij}^1 \frac{T}{1000}\right)$$

Table S11. Regressed parameters in [SI] for [EMIM][TfO] (i) and CH_4 (j) with CPA and PC-SAFT models with different associative schemes of the ionic liquid for β^{AB} e K^{AB} equal to one.

					CPA					
Schemes	NA*		1A		2B		3B		4C	
Parameters	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1
1p	0.08275	0	0.07917	0	0.07381	0	0.07381	0	0.06022	0
2p	0.16636	-0.07751	0.16935	-0.08361	0.16675	-0.08619	0.16675	-0.08619	0.21052	-0.13943
					PC-SAFT					
Schemes	NA*		1A		2B		3B		4C	
Parameters	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1
1p	-0.10359	0	-0.10292	0	-0.10271	0	-0.10271	0	-0.10203	0
2p	0.06731	-0.09611	0.04432	-0.15865	0.02092	-0.06952	0.02092	-0.06953	-0.02364	-0.04409

* NA: Non-associative. CPA: $k_{ij} = k_{ij}^0 + k_{ij}^1 \frac{T}{T_{ref} = 298.15K}$. PC-SAFT: $k_{ij} = k_{ij}^0 + \frac{k_{ij}^1}{T_r}$.

Table S12. Regressed parameters in [SI] for [EMIM][TfO] (i) and CO_2 (j) with CPA and PC-SAFT models with different associative schemes of the ionic liquid for β^{AB} e K^{AB} equal to one.

					CPA					
Schemes	NA*		1A		2B		3B		4C	
Parameters	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1
1p	0.03019		0,01586	0	-0,00067	0	-0,00067	0	-0,04226	0
2p	0.19635	-0.15320	0,20084	-0,17057	0,20893	-0,19330	0,20893	-0,19330	0,24176	-0,26203
					PC-SAFT					
Schemes	NA*		1A		2B		3B		4C	
Parameters	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1
1p	0,01917	0	0,00925	0	-0,00031	0	-0,00031	0	-0,01799	0
2p	0,04450	-0,02742	0,02403	-0,01601	0,00329	-0,00390	0,00329	-0,00390	-0,03734	0,02098

* NA: Non-associative. CPA: $k_{ij} = k_{ij}^0 + k_{ij}^1 \frac{T}{T_{ref} = 298.15K}$. PC-SAFT: $k_{ij} = k_{ij}^0 + \frac{k_{ij}^1}{T_r}$.

Table S13. Regressed parameters in [SI] for [EMIM][TfO] (i) and CO_2 (j) with CPA and PC-SAFT models with different associative parameters of the ionic liquid for NA and 2B scheme.

					CPA					
Schemes	NA*		β^{AB}=1		β^{AB}=0.1		β^{AB}=0.001		β^{AB}=0.00001	
Parameters	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1
1p	0.03019	0	-0.00067	0	-0.00067	0	-0.00067	0	-0.00066	0
2p	0.19635	-0.15320	0.20893	-0.19330	0.20893	-0.19330	0.20891	-0.19328	0.20869	-0.19307
					PC-SAFT					
Schemes	NA*		K^{AB}=1		K^{AB}=0.1		K^{AB}=0.001		K^{AB}=0.00001	
Parameters	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1
1p	0.01917	0	-0.00031		-0.00033	0	-0.00032	0	-0.00032	0
2p	0.04450	-0.02742	0.00329	-0.00390	0.00326	-0.00390	0.00327	-0.00390	0.00328	-0.00390

* NA: Non-associative. CPA: $k_{ij} = k_{ij}^0 + k_{ij}^1 \frac{T}{T_{ref} = 298.15K}$. PC-SAFT: $k_{ij} = k_{ij}^0 + \frac{k_{ij}^1}{T_r}$.

Table S14. Regressed parameters in [SI] for [EMIM][TfO] (i) and H_2S (j) with CPA and PC-SAFT models with different associative schemes of the ionic liquid for β^{AB} e K^{AB} equal to one.

					CPA					
Schemes	NA*		1A		2B		3B		4C	
Parameters	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1
1p	-0.11494	0	0.03387	0	0.04658	0	NR**	NR**	0.10690	0
2p	0.16053	-0.25611	-0.13650	0.15839	-0.02072	0.06258	NR**	NR**	-0.00065	0.10010
					PC-SAFT					
Schemes	NA*		1A		2B		3B		4C	
Parameters	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1
1p	-0.00577	0	-0.00913	0	-0.01831	0	0.53917	0	-0.03218	0
2p	-0.01078	0.00536	-0.01923	0.01083	-0.03301	0.01577	0.35696	0.20056	-0.05642	0.02605

* NA: Non-associative. ** NR: No results. CPA: $k_{ij} = k_{ij}^0 + k_{ij}^1 \frac{T}{T_{ref} = 298.15K}$. PC-SAFT: $k_{ij} = k_{ij}^0 + \frac{k_{ij}^1}{T_r}$.

Table S15. Regressed parameters in [SI] for [EMIM][TfO] (i) and H_2S (j) with CPA and PC-SAFT models with different associative parameters of the ionic liquid for NA and 2B scheme.

					CPA					
Schemes	NA*		β^{AB}=1		β^{AB}=0.1		β^{AB}=0.001		β^{AB}=0.00001	
Parameters	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1
1p	-0.11494	0	0.04658	0	0.04658	0	0.04658	0	0.04656	0
2p	0.16053	-0.25611	-0.02072	0.06258	-0.02072	0.06257	-0.02069	0.06255	-0.02049	0.06234
					PC-SAFT					
Schemes	NA*		K^{AB}=1		K^{AB}=0.1		K^{AB}=0.001		K^{AB}=0.00001	
Parameters	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1
1p	-0.00577	0	-0.01831	0	-0.01833	0	-0.01832	0	-0.01832	0
2p	-0.01078	0.00536	-0.03301	0.01577	-0.03302	0.01576	-0.03302	0.01577	-0.03302	0.01576

Table S16. Regressed parameters in [SI] for [OMIM][NTf_2] (i) and CO_2 (j) with CPA and PC-SAFT models with different associative schemes of the ionic liquid for β^{AB} e K^{AB} equal to one.

					CPA					
Schemes	NA*		1A		2B		3B		4C	
Parameters	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1
1p	-0.12307	0	-0.14721	0	-0,17441	0	-0,17441	0	-0,24057	
2p	0.34902	-0.42693	0.40481	-0.49940	0,47435	-0,58717	0,47435	-0,58717	0,67256	-0,82728
					PC-SAFT					
Schemes	NA*		1A		2B		3B		4C	
Parameters	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1
1p	0.00989	0	0.00256	0	-0,00464	0	-0,00464	0	-0,01899	0
2p	-0.05048	0.06685	-0.06784	0.07799	-0,08525	0,08932	-0,08525	0,08932	-0,12003	0,11202

* NA: Non-associative. CPA: $k_{ij} = k_{ij}^0 + k_{ij}^1 \frac{T}{T_{ref} = 298.15K}$. PC-SAFT: $k_{ij} = k_{ij}^0 + \frac{k_{ij}^1}{T_r}$.

Table S17. Regressed parameters in [SI] for [OMIM][NTf_2] (i) and H_2S (j) with CPA and PC-SAFT models with different associative schemes of the ionic liquid for β^{AB} e K^{AB} equal to one.

					CPA					
Schemes	NA*		1A		2B		3B		4C	
Parameters	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1
1p	-0.26137	0	-0,00097		-0.01580	0	NR**	NR**	0,05242	0
2p	0.40446	-0.60235	0,06721	-0,06165	0.18585	-0.18257	NR**	NR**	0,21765	-0,14976
					PC-SAFT					
Schemes	NA*		1A		2B		3B		4C	
Parameters	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1	k_{ij}^0	k_{ij}^1
1p	-0.00103	0	-0,00199	0	-0.00755	0	0,76330	0	-0,01547	0
2p	-0.08395	0.09168	-0,09157	0,09906	-0.10371	0.10634	1,13283	-0,39925	-0,12417	0,12026

* NA: Non-associative. ** NR: No results. CPA: $k_{ij} = k_{ij}^0 + k_{ij}^1 \frac{T}{T_{ref} = 298.15K}$. PC-SAFT: $k_{ij} = k_{ij}^0 + \frac{k_{ij}^1}{T_r}$.

Supplementary E2. Properties calculation of pure ILs

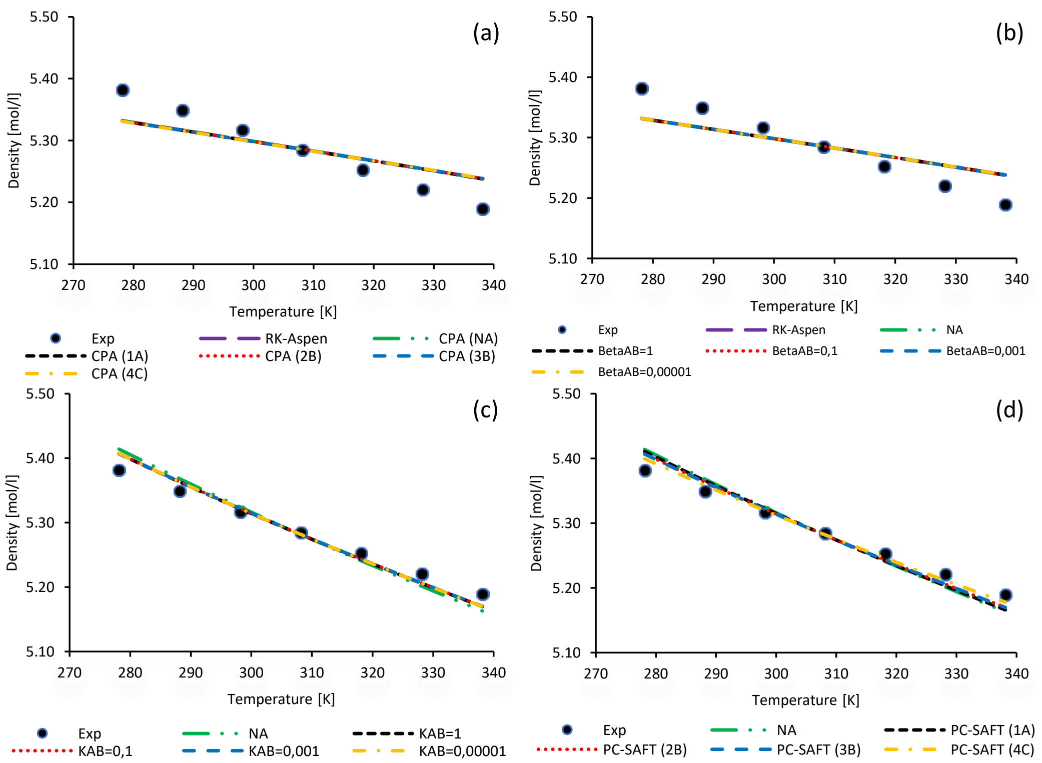

Figure S10. Density vs temperature results for [EMIM][TfO]; (a) Results for the RK-Aspen model and the non-associative CPA and with different associative schemes; (b) Results for different associative parameters for CPA EoS; (c) Results for different associative parameters for PC-SAFT EoS; (d) Results for the non-associative PC-SAFT and with different associative schemes. Experimental data from Vercher et al. [9].

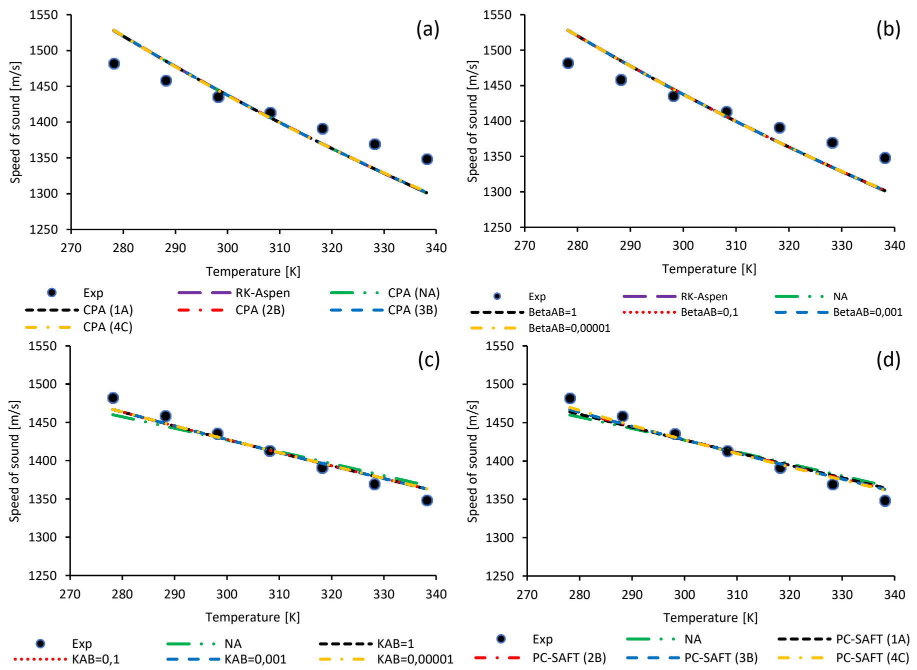

Figure S11. Speed of sound vs temperature results for [EMIM][TfO]: (a) Results for the RK-Aspen model and the non-associative CPA and with different associative schemes; (b) Results for different associative parameters for CPA EoS; (c) Results for different associative parameters for PC-SAFT EoS; (d) Results for the non-associative PC-SAFT and with different associative schemes. Experimental data from Vercher et al. [9].

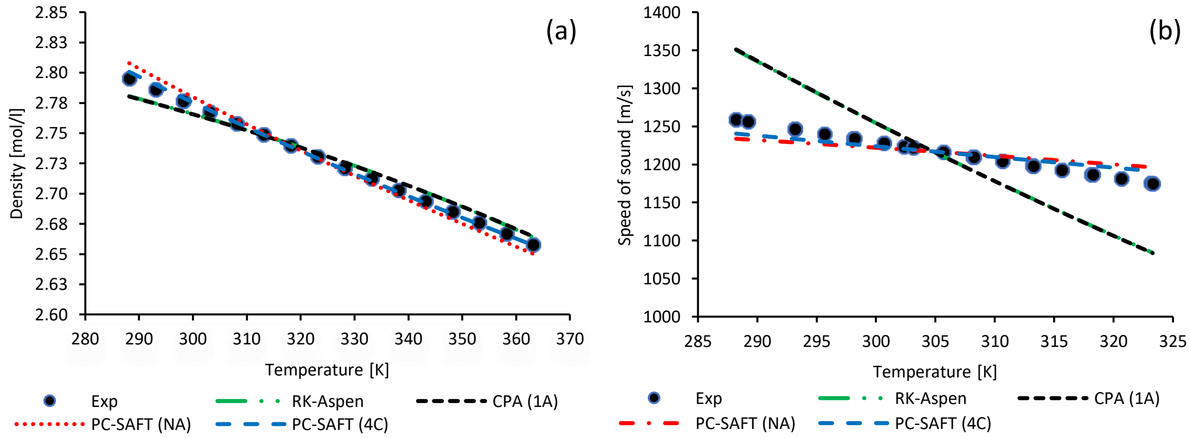

Figure S12. Density and speed of sound results for the RK-Aspen, CPA, and PC-SAFT models. Experimental data from Zorębski et al. [10].

Supplementary E3. Methane (CH_4) with [EMIM][TfO] results

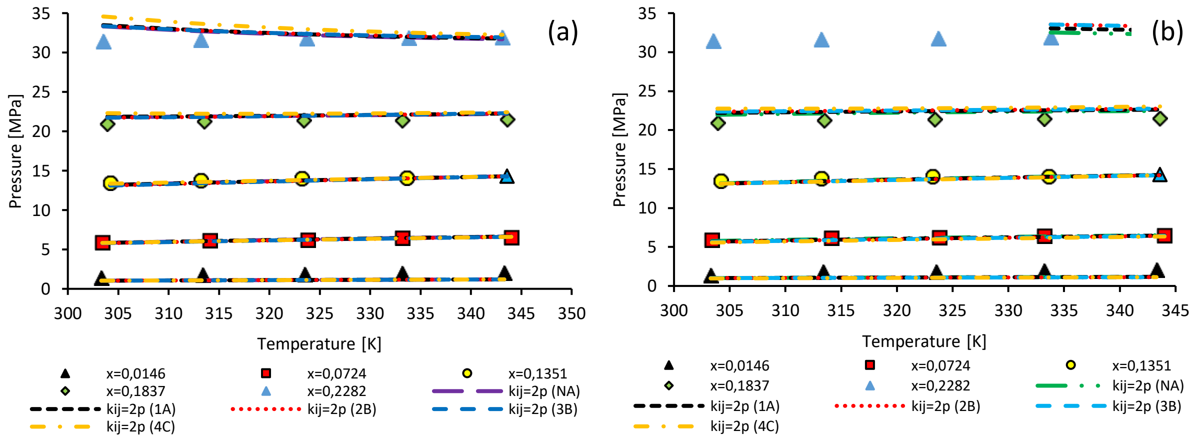

Figure S13. P-T results for CH_4 and [EMIM][TfO]: (a) Results for CPA EoS with k_{ij}=2p for different associative schemes; (b) Results for PC-SAFT EoS with k_{ij}=2p for different associative schemes. Experimental data from Lee [11].

Table S18. Deviations in pressure for CH_4 and [EMIM][TfO] using the RK-Aspen model.

x_{CH_4}	k_{ij}=0	k_{ij}=2p	k_{ij}=4p
0.0146	48.16	41.12	40.78
0.0724	20.60	9.26	2.79
0.1351	26.03	8.39	1.18
0.1837	27.26	11.82	2.68
0.2282	32.15	6.93	2.89
Average deviation (AARD)	23.02	11.50	8.54

$$AARD(\%) = \frac{1}{n}\sum_{i=1}^{n}\left|\frac{p_i^{exp} - p_i^{cal}}{p_i^{exp}}\right| 100$$

Table S19. Deviations in pressure for CH_4 and [EMIM][TfO] using the CPA and PC-SAFT EoS.

	CPA														
	k_{ij}=0					k_{ij}=1p					k_{ij}=2p				
x_{CH_4}	NA	1A	2B	3B	4C	NA	1A	2B	3B	4C	NA	1A	2B	3B	4C
0.0146	59.21	58.22	57.01	57.01	53.71	40.48	40.70	41.05	41.05	41.21	41.40	41.59	41.76	41.76	42.06
0.0724	38.06	36.31	34.17	34.17	28.39	4.18	4.08	4.43	4.43	4.96	1.49	1.37	1.89	1.89	1.41
0.1351	43.80	41.90	39.56	39.56	33.17	5.20	5.37	5.91	5.91	5.91	2.23	2.30	2.75	2.75	1.67
0.1837	46.06	43.89	41.22	41.22	33.75	6.93	7.26	7.46	7.46	9.99	4.14	4.33	3.79	3.79	6.46
0.2282	50.83	48.47	45.55	45.55	37.24	3.22	3.80	4.26	4.25	7.53	5.99	6.49	6.10	6.10	9.96
AARD	42.42	40.49	38.09	38.09	31.35	9.60	9.77	9.91	9.91	10.78	8.99	9.12	9.24	9.24	9.74
	PC-SAFT														
	k_{ij}=-0.1					k_{ij}=1p					k_{ij}=2p				
x_{CH_4}	NA	1A	2B	3B	4C	NA	1A	2B	3B	4C	NA	1A	2B	3B	4C
0.0146	35.78	37.29	38.31	38.31	40.16	38.11	39.13	39.99	39.99	41.38	38.47	39.40	40.19	40.19	41.48
0.0724	7.68	5.98	4.90	4.90	3.61	7.14	6.12	5.50	5.50	4.81	1.34	2.33	3.17	3.17	4.51
0.1351	9.86	7.91	6.37	6.37	3.70	8.99	7.61	6.30	6.30	3.87	1.49	1.71	1.87	1.87	2.06
0.1837	27.33	26.62	12.67	12.67	11.28	12.18	10.78	9.41	9.41	7.67	4.31	5.07	5.79	5.79	7.09
0.2282	62.64	61.69	61.17	61.17	80.39	64.79	63.49	62.21	62.21	60.78	60.59	61.27	61.89	61.89	81.38
AARD *	20.16	19.45	15.56	15.56	14.69	16.60	15.91	15.30	15.30	14.43	11.40	12.13	12.76	12.76	13.79

* These data were performed disregarding x_{CH_4}=0.2282.

Supplementary E4. Carbon Dioxide (CO_2) with ionic liquids results

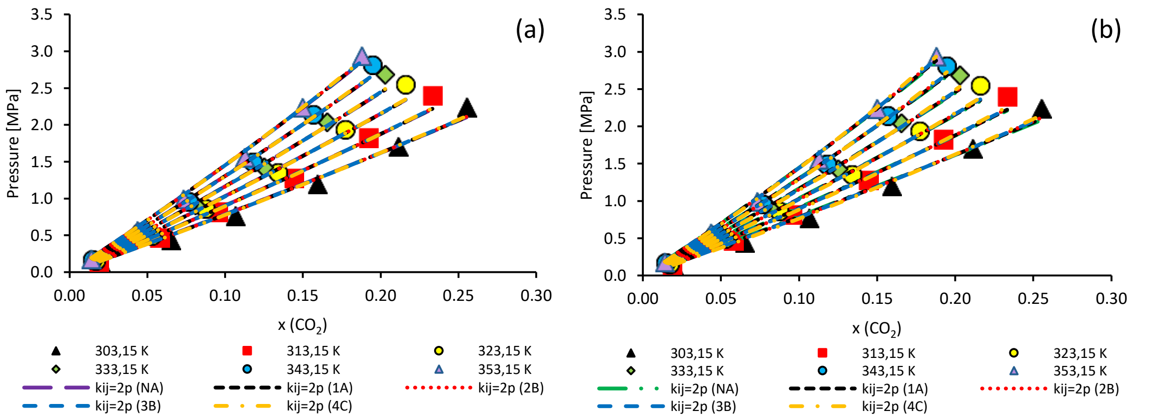

Figure S14. P-x results for CO_2 and [EMIM][TfO]: (a) Results for CPA EoS with k_{ij}=2p for different associative schemes; (b) Results for PC-SAFT EoS with k_{ij}=2p for different associative schemes. Experimental data from Nematpour et al. [12].

Table S20. Deviations in pressure for CO_2 and [EMIM][TfO] using the RK-Aspen model.

Temperature [K]	CO_2		
	k_{ij}=0	k_{ij}=2p	k_{ij}=4p
303.15	10.50	5.05	3.16
313.15	8.25	4.61	1.38
323.15	5.39	3.31	2.26
333.15	3.82	2.53	2.45
343.15	4.98	4.05	1.41
353.15	9.36	8.81	2.38
AARD	7.05	4.69	2.17

Table S21. Deviations in pressure for CO_2 and [EMIM][TfO] using the CPA and PC-SAFT EoS.

	CPA														
	k_{ij}=0					k_{ij}=1p					k_{ij}=2p				
Temperature [K]	NA	1A	2B	3B	4C	NA	1A	2B	3B	4C	NA	1A	2B	3B	4C
303.15	18.71	11.12	4.81	4.81	21.51	5.22	5.01	4.79	4.79	5.65	7.95	7.73	7.52	7.52	7.12
313.15	17.08	9.46	4.80	4.80	23.47	5.24	4.97	4.78	4.78	4.66	6.51	6.30	6.08	6.08	5.65
323.15	14.90	7.19	5.34	5.34	26.25	5.59	5.39	5.20	5.20	4.81	5.61	5.42	5.22	5.22	4.81
333.15	12.21	4.64	6.24	6.24	29.75	5.36	5.94	5.97	5.97	6.25	4.85	4.67	4.49	4.49	4.12
343.15	8.27	3.71	9.39	9.39	35.11	8.15	8.51	9.01	9.01	10.62	4.75	4.59	4.42	4.42	4.10
353.15	3.99	5.36	14.58	14.58	41.36	12.74	13.35	14.20	14.20	16.84	5.15	5.01	4.87	4.87	4.63
AARD	12.53	6.91	7.53	7.53	29.57	7.15	7.19	7.33	7.33	8.14	5.81	5.62	5.43	5.43	5.07
	PC-SAFT														
	k_{ij}=0					k_{ij}=1p					k_{ij}=2p				
Temperature [K]	NA	1A	2B	3B	4C	NA	1A	2B	3B	4C	NA	1A	2B	3B	4C
303.15	19.01	7.34	7.61	7.61	34.89	10.79	8.99	7.26	7.26	4.31	8.82	7.86	6.99	6.99	5.45
313.15	21.18	9.49	5.64	5.64	31.57	7.64	6.51	5.46	5.46	3.53	7.16	6.24	5.39	5.39	3.86
323.15	22.54	11.03	4.55	4.55	29.66	5.89	5.11	4.38	4.38	3.05	5.91	5.12	4.38	4.38	3.05
333.15	23.23	11.79	3.62	3.62	28.90	4.42	3.92	3.46	3.46	2.64	4.83	4.15	3.52	3.52	2.46
343.15	22.66	11.10	3.37	3.37	30.29	3.70	3.44	3.22	3.22	3.00	4.44	3.86	3.32	3.32	2.32
353.15	21.48	9.71	3.73	3.73	32.70	3.53	3.49	3.49	3.49	5.23	4.56	4.08	3.72	3.72	3.08
AARD	21.68	10.08	4.75	4.75	31.33	5.99	5.24	4.54	4.54	3.63	5.95	5.22	4.55	4.55	3.37

Table S22. Deviations in pressure for CO_2 and [OMIM][NTf$_2$] using the RK-Aspen model.

Temperature [K]	CO_2		
	k_{ij}=0	k_{ij}=2p	k_{ij}=4p
303.15	57.81	17.39	1.44
313.15	63.18	11.26	1.00
323.15	68.08	5.23	1.01
333.15	73.25	1.75	1.06
343.15	77.87	7.57	0.89
353.15	83.79	15.08	1.32
AARD	70.66	9.71	1.12

Table S23. Deviations in pressure for CO_2 and [OMIM][NTf$_2$] using the CPA and PC-SAFT EoS.

	CPA														
	k_{ij}=0					k_{ij}=1p					k_{ij}=2p				
Temperature [K]	NA	1A	2B	3B	4C	NA	1A	2B	3B	4C	NA	1A	2B	3B	4C
303.15	53.56	66.11	80.48	80.47	116.35	16.68	18.60	20.75	20.75	25.91	7.48	7.42	7.36	7.36	7.30
313.15	58.43	71.62	86.81	86.81	125.15	10.71	11.98	13.41	13.41	16.90	6.31	6.21	6.10	6.10	5.88
323.15	62.73	76.53	92.51	92.50	133.25	6.69	6.84	7.00	7.00	7.67	5.77	5.70	5.62	5.62	5.48
333.15	67.20	81.64	98.45	98.44	141.77	5.44	5.38	5.34	5.34	5.30	5.12	5.04	4.97	4.97	4.83
343.15	71.08	86.13	103.75	103.74	126.82	7.69	8.41	9.27	9.27	12.16	4.65	4.57	4.48	4.48	4.33
353.15	76.15	91.97	110.58	110.57	159.61	13.12	15.06	17.36	17.36	23.47	3.72	3.64	3.58	3.58	3.48
AARD	64.86	79.00	95.43	95.43	133.82	10.06	11.04	12.19	12.19	15.24	5.51	5.43	5.35	5.35	5.22
	PC-SAFT														
	k_{ij}=0					k_{ij}=1p					k_{ij}=2p				
Temperature [K]	NA	1A	2B	3B	4C	NA	1A	2B	3B	4C	NA	1A	2B	3B	4C
303.15	17.80	10.36	5.32	5.33	15.06	8.12	7.77	8.31	8.31	10.22	7.34	6.30	5.36	5.36	3.47
313.15	16.10	8.45	3.82	3.82	17.81	6.40	5.99	6.06	6.06	7.24	5.52	4.61	3.77	3.77	2.19
323.15	14.26	6.38	3.57	3.57	20.69	5.07	4.58	4.15	4.15	4.14	4.65	3.88	3.30	3.30	2.13
333.15	11.86	3.96	5.01	5.01	24.38	3.61	2.91	2.25	2.25	1.11	3.68	3.06	2.55	2.55	1.58
343.15	9.30	2.27	8.11	8.11	28.23	3.52	3.15	3.03	3.03	3.50	2.91	2.28	1.79	1.79	0.92
353.15	5.55	3.31	12.73	12.73	33.89	5.54	6.28	7.13	7.13	8.88	1.86	1.41	1.12	1.12	1.68
AARD	12.48	5.79	6.43	6.43	23.34	5.36	5.11	5.15	5.15	5.85	4.33	3.59	3.00	3.00	2.00

Supplementary E5. Hydrogen sulfide (H_2S) with ionic liquids results

Table S24. Deviations in pressure for H_2S and [EMIM][TfO] using the RK-Aspen model.

Temperature [K]	H_2S		
	k_{ij}=0	2p	4p
303.15	18.90	2.52	2.79
313.15	18.26	2.29	2.30
323.15	19.15	1.34	1.14

333.15	18.12	1.80	1.46
343.15	18.25	2.01	1.09
353.15	18.61	3.01	1.65
AARD	18.55	2.16	1.74

Table S25. Deviations in pressure for H_2S and [EMIM][TfO] using the CPA e PC-SAFT EoS.

	CPA														
	k_{ij}=0					1p					2p				
Temperature [K]	NA	1A	2B	3B	4C	NA	1A	2B	3B	4C	NA	1A	2B	3B	4C
303.15	165.34	15.79	11.54	94.90	30.25	34.13	2.85	15.11	DU	21.90	43.79	3.86	13.30	DU	19.05
313.15	162.19	17.95	13.15	96.41	31.32	33.98	2.94	12.52	DU	18.15	38.15	3.80	11.80	DU	17.05
323.15	162.63	19.19	13.68	98.22	31.54	36.00	3.38	11.36	DU	16.03	34.71	2.90	11.57	DU	16.44
333.15	158.48	21.38	15.39	99.99	32.68	35.52	6.40	9.16	DU	12.92	29.40	3.49	9.82	DU	14.03
343.15	157.62	22.48	15.96	100.00	32.91	37.00	8.26	7.98	DU	11.12	25.90	3.26	9.08	DU	12.88
353.15	155.59	23.53	16.63	100.00	33.23	38.71	10.06	5.89	DU	8.48	21.74	3.95	7.33	DU	10.77
AARD	160.31	20.05	14.39	98.25	31.99	35.89	5.65	10.34	DU	14.77	32.28	3.54	10.48	DU	15.04
	PC-SAFT														
	k_{ij}=0					1p					2p				
Temperature [K]	N	1A	2B	3B	4C	NA	1A	2B	3B	4C	NA	1A	2B	3B	4C
303.15	35.92	37.32	50.71	94.26	71.31	26.49	21.78	16.96	32.71	8.92	26.89	22.54	18.03	41.85	10.48
313.15	31.14	33.14	46.53	96.06	67.77	22.44	18.54	14.49	38.57	7.71	22.57	18.81	14.88	40.14	8.28
323.15	28.34	30.88	44.41	98.01	66.42	20.14	16.90	13.49	39.39	7.72	20.07	16.76	13.31	39.88	7.51
333.15	23.84	26.85	40.31	99.51	62.73	16.21	13.63	10.87	41.78	6.20	15.97	13.16	10.25	37.89	5.51
343.15	21.21	24.66	38.21	99.70	61.24	13.73	11.69	9.47	46.41	5.78	13.35	11.01	8.61	37.81	4.49
353.15	18.47	22.33	35.92	99.68	59.49	10.53	8.98	7.65	38.57	5.78	10.16	8.19	6.14	27.26	3.09
AARD	26.49	29.20	42.68	97.87	64.83	18.26	15.25	12.16	39.57	7.02	18.17	15.08	11.87	37.47	6.56

* DU: Data Unavailable

Table S26. Deviations in pressure for H_2S and [OMIM][NTf$_2$] using the RK-Aspen model.

Temperature [K]	H_2S		
	k_{ij}=0	2p	4p
303.15	38.43	14.98	4.95
313.15	48.52	9.45	4.33
323.15	53.39	4.84	3.78
333.15	58.17	4.07	3.57
343.15	70.74	8.93	2.17
353.15	75.83	14.93	2.24
AARD	57.51	9.53	3.51

Table S27. Deviations in pressure for H_2S and [OMIM][NTf$_2$] using the CPA e PC-SAFT EoS

	CPA														
	k_{ij}=0					1p					2p				
Temperature [K]	NA	1A	2B	3B	4C	NA	1A	2B	3B	4C	NA	1A	2B	3B	4C
303.15	154.93	14.24	2.09	74.02	22.92	24.37	14.08	5.39	DU	5.47	15.55	14.08	2.11	DU	2.90
313.15	175.61	12.35	3.64	83.71	21.38	15.92	12.22	3.73	DU	4.15	13.75	12.22	1.98	DU	3.66
323.15	179.48	11.88	4.15	86.58	19.83	12.35	11.76	2.44	DU	3.51	12.21	11.76	1.74	DU	3.37
333.15	182.87	11.05	5.12	89.20	18.24	11.63	10.93	1.80	DU	3.50	11.23	10.93	2.12	DU	3.55
343.15	203.60	9.16	8.62	96.82	14.05	13.50	8.99	3.23	DU	4.01	9.40	8.99	1.40	DU	3.49
353.15	205.63	9.01	10.39	98.26	11.65	18.12	8.85	4.96	DU	4.79	8.50	8.85	1.51	DU	3.17
AARD	183.69	11.28	5.67	88.10	18.01	15.98	11.14	3.59	DU	4.24	11.77	11.14	1.81	DU	3.36
	PC-SAFT														
	k_{ij}=0					1p					2p				
Temperature [K]	NA	1A	2B	3B	4C	NA	1A	2B	3B	4C	NA	1A	2B	3B	4C
303.15	9.38	8.35	5.61	79.32	8.54	10.52	10.54	10.53	DU	10.11	9.08	7.52	5.92	DU	3.57
313.15	6.83	5.38	6.10	87.48	12.53	7.03	6.76	6.81	DU	6.63	7.34	5.97	4.71	DU	3.07
323.15	5.68	4.46	6.62	89.62	15.44	5.56	4.65	4.43	DU	3.74	5.78	4.43	3.33	DU	2.74
333.15	5.08	4.48	8.23	91.62	18.61	4.87	3.67	2.97	DU	2.71	4.75	3.77	3.25	DU	2.88
343.15	5.82	6.58	13.50	97.70	25.47	5.16	4.77	4.67	DU	5.33	3.70	2.76	1.85	DU	1.70
353.15	7.92	9.34	17.17	98.71	29.89	6.98	7.13	7.80	DU	9.60	2.98	2.39	1.82	DU	2.15
AARD	6.78	6.43	9.54	90.74	18.41	6.69	6.25	6.20	DU	6.35	5.60	4.47	3.48	DU	2.68

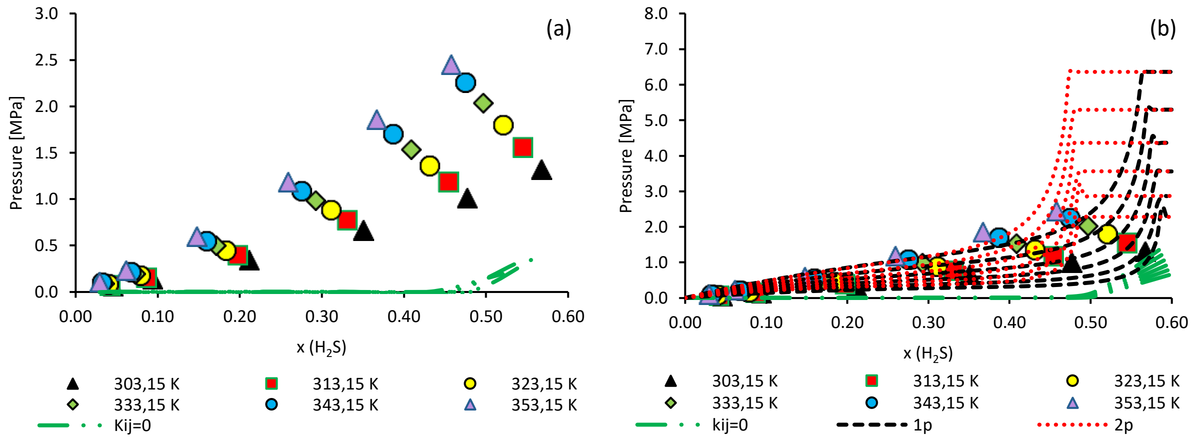

Figure S15. P-x results for H_2S and [EMIM][TfO]: (a) CPA EoS with k_{ij} =0 for 3B associative scheme; (b) PC-SAFT EoS with k_{ij} =0, 1p e 2p for 3B associative scheme. Experimental data from Nematpour et al. [12].

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