Supporting Information

Predicting the Thermodynamics of Ionic Liquids: What to Expect from PC-SAFT and COSMO-RS?

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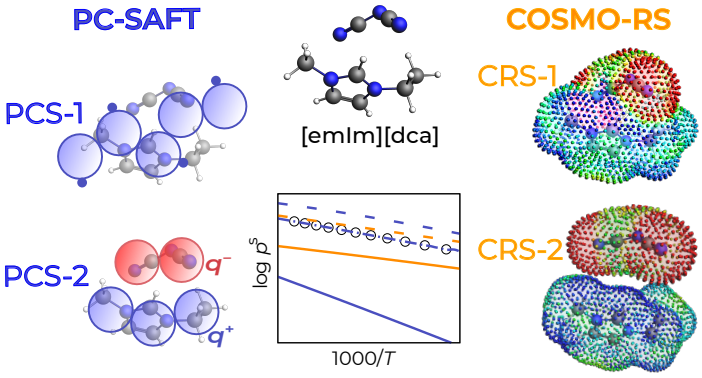

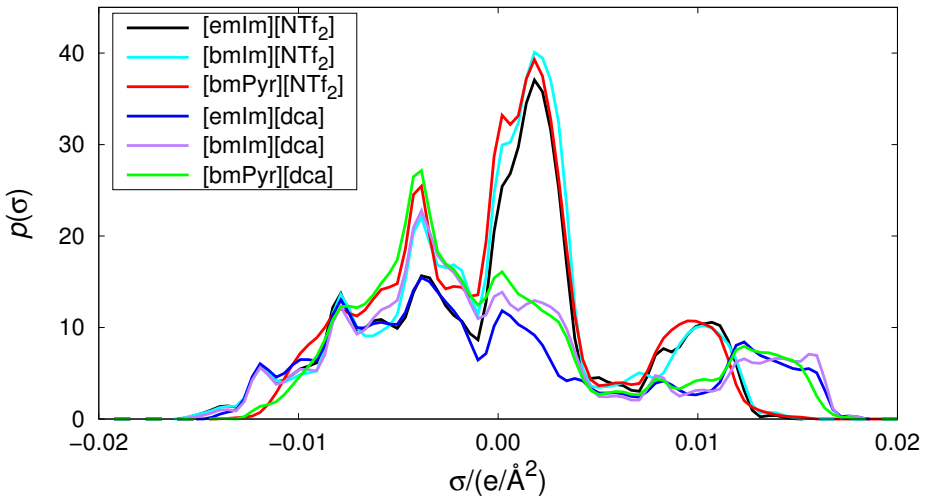

Figure S1: Calculated σ-profiles for the IL pairs considered in this work for calculations with COSMO-RS and Approach 1 (CRS-1).

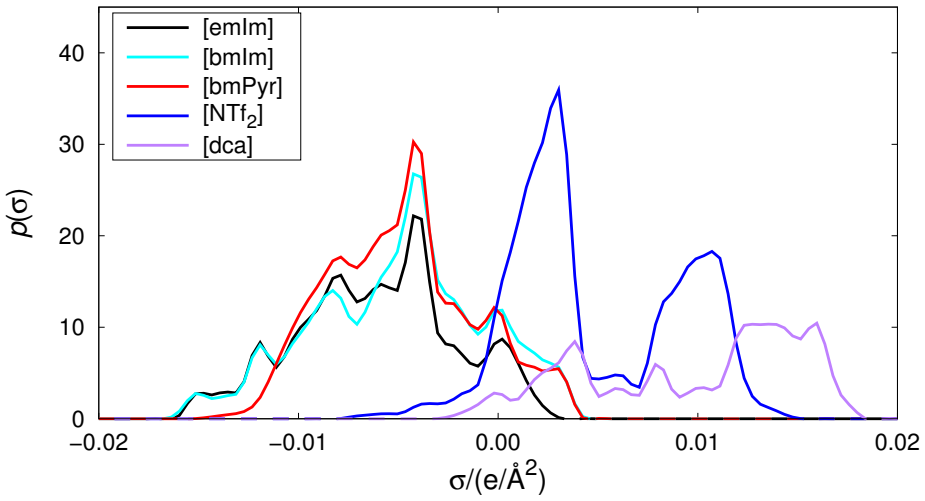

Figure S2: Calculated σ-profiles for the individual IL-forming ions considered in this work for calculations with COSMO-RS and Approach 2 (CRS-2).

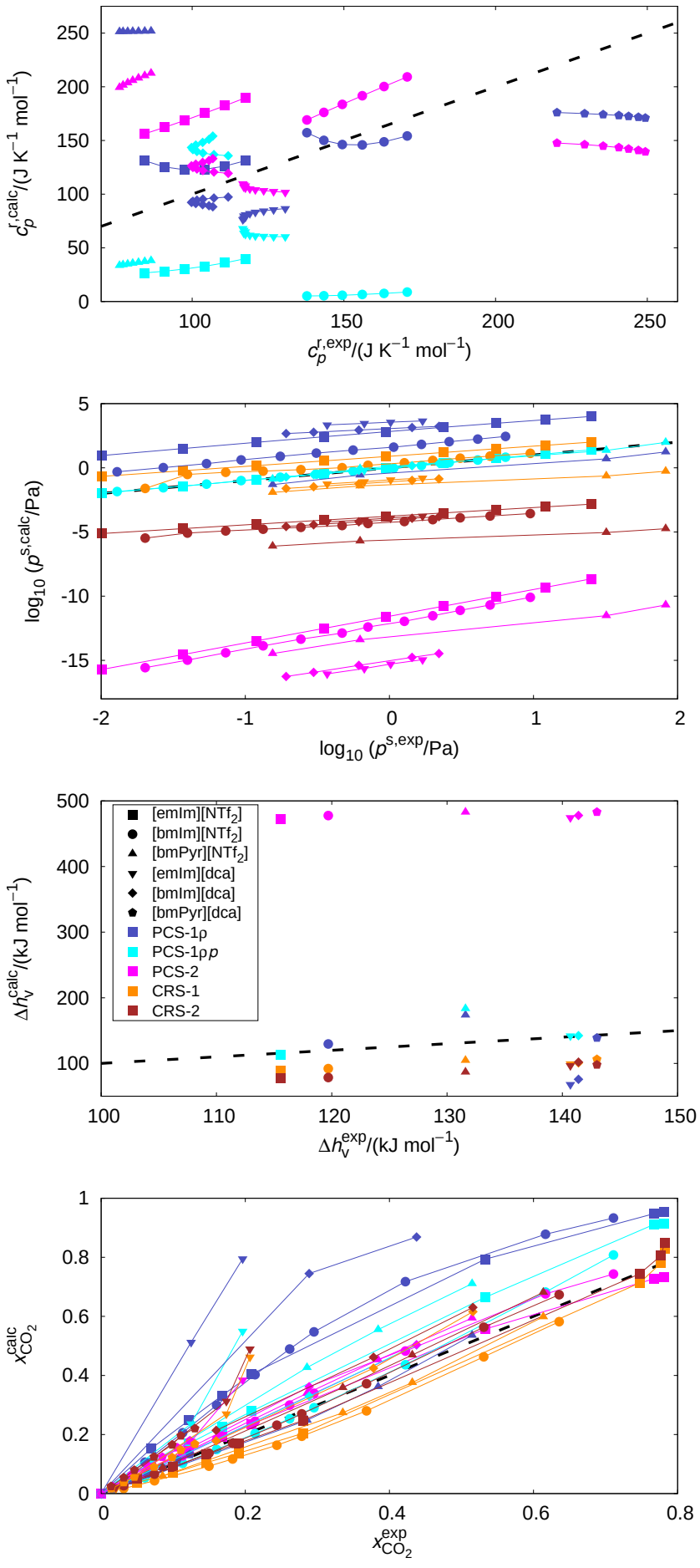

Figure S3: Diagonal comparison of experimental and calculated data. The lines are to guide the eyes.

Table S1: In addition to the PCS-1 parameters considered in the main article, we also evaluated the performance of some other existing PC-SAFT parameters for ILs (considering the electroneutral supermolecule approach PCS-1) available in the literature. These existing sets together with their statistical deviations are provided below.

m	σ'/Å	(u/k_B)/K	(ε^{as}/k_B)/K	κ^{as}	N^{as}	Fitted to	Source	100· AARD(c_p^r)	MALD(p^s)	100·AARD(Δh_v)	100·AARD(x_{CO_2})
						[emIm][NTf_2]					
8.6100	3.5700	331.00	5000.0[a]	0.1[a]	2 (1, 1, 0)	ρ	Ji et al. [1]	91 (+)	0.9 (−)	46 (+)	9.1 (+)
5.6700	4.2800	457.40	3450.00[a]	0.00225[a]	3 (2, 1, 0)	ρ, p^s	Chen et al. [2]	61 (+)	0.3 (−)	35 (+)	53 (+)
6.5240	3.9733	342.09	4016.6	0.11	2 (1, 1, 0)	ρ, p^s	Bülow et al. [3]	45 (+)	1.1 (+)	16 (+)	50 (+)
						[bmIm][NTf_2]					
10.180	3.5000	299.00	5000.0[a]	0.1[a]	2 (1, 1, 0)	ρ	Ji et al. [1]	33 (+)	0.8 (−)	43 (+)	9.2 (+)
5.7200	4.3700	458.90	3450.0[a]	0.00225[a]	3 (2, 1, 0)	ρ, p^s	Chen et al. [2]	5.5 (+)	0.2 (−)	32 (+)	71 (+)
						[emIm][dca]					
3.9100	4.0900	358.99	5000.0[a]	0.1[a]	8 (4, 4, 0)	ρ, $\gamma^{\infty,b}$	Carneiro et al. [4]	50 (−)	6.1 (−)	70 (+)	74 (+)
						[bmIm][dca]					
7.4412	3.4140	290.74	2276.4	0.0797	6 (3, 3, 0)	ρ, p^s	Paduszyński et al. [5]	69 (+)	0.01 (−)	0.1 (−)	6.2 (−)
2.8670	4.9890	518.88	5000.0[a]	0.1[a]	10 (5, 5, 0)	ρ, x^c	Carneiro et al. [4]	53 (−)	5.4 (−)	109 (+)	101 (+)

[a] Kept fixed by the authors during the parameter regression. [b] Infinite-dilution activity coefficient of 1-propanol in [emim][dca]. [c] Solubility of xylitol in [bmIm][dca].

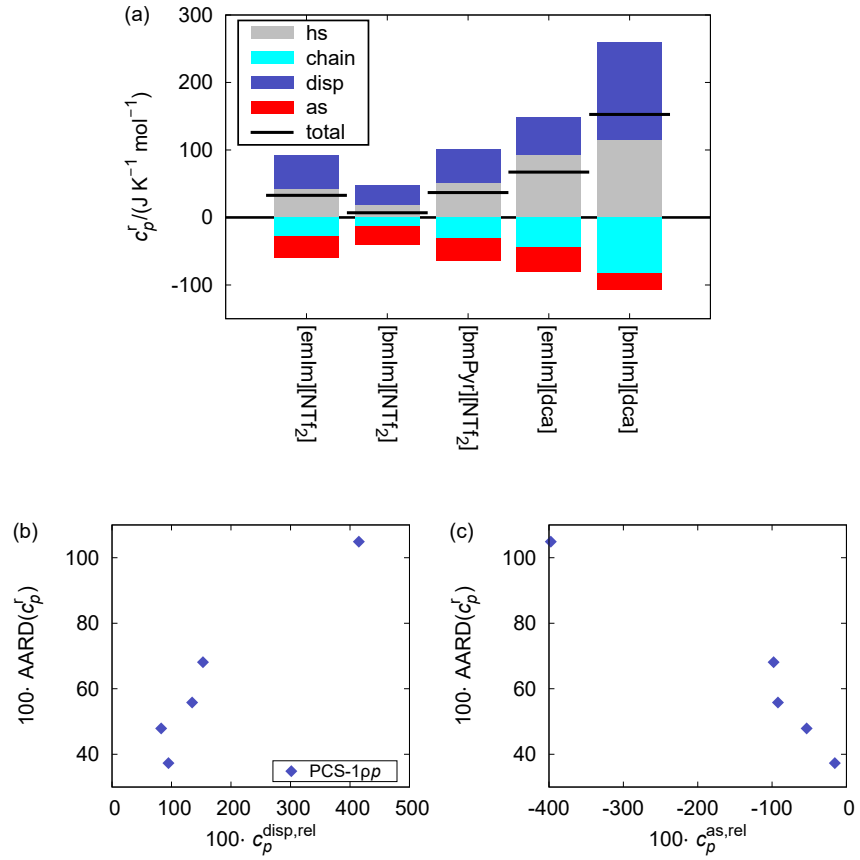

Figure S4: Analysis of the correlation between the error in c_p^{r} and contributions of the individual terms of the PC-SAFT EOS for the five ILs considered in PCS-1ρp: (a) the individual contributions to c_p^{r}; (b) correlation of the relative influence (in %) of dispersions and the error; and (c) correlation of the relative influence (in %) of associations and the error. The data corresponds to $T = 300$ K.

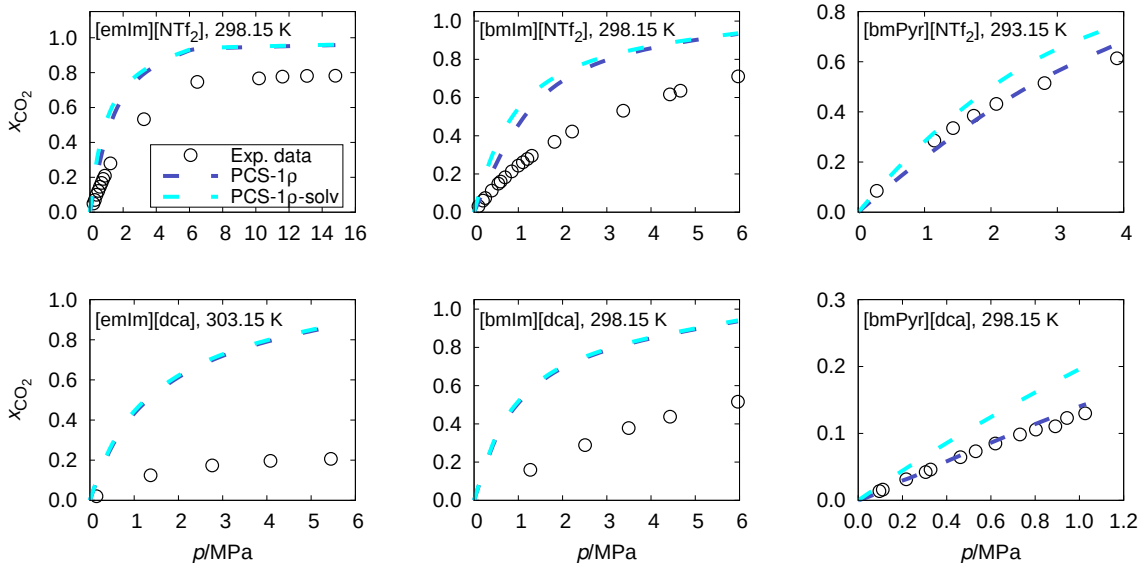

Figure S5: Comparison of PCS-1ρ results for the solubility of CO_2 in the ILs obtained (i) without (PCS-1ρ) and (ii) with (PCS-1ρ-solv) the solvation, i.e., the IL–CO_2 cross associations.

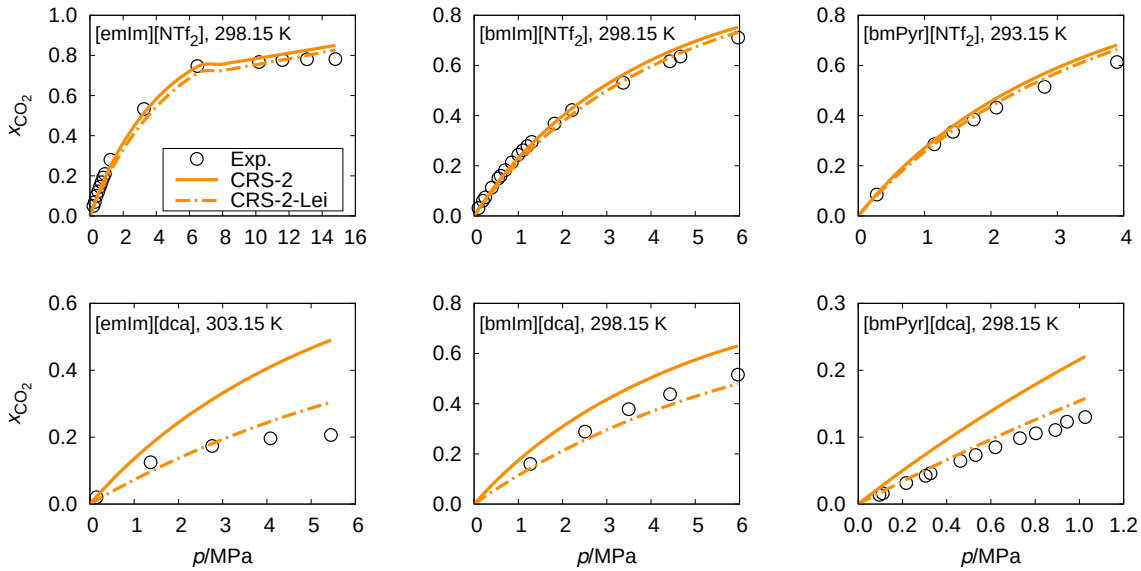

Figure S6: Comparison of CRS-2 results for the solubility of CO_2 in the ILs obtained using (i) the standard intrinsic model parameters (CRS-2) and (ii) the intrinsic parameters by Lei et al. [6] (CRS-2-Lei) reevaluated specifically for IL mixtures.

References

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