

Supporting information

**High pressure separation of greenhouse gases from air with
1-ethyl-3-methylimidazolium methyl-phosphonate**

Luís M. C. Pereira[†], Mariana B. Oliveira[†], Ana M. A. Dias[‡], Felix Llovell[‡], Lourdes F. Vega^{‡,§}, Pedro
J. Carvalho[†] and João A. P. Coutinho^{†,*}

[†]CICECO, Departamento de Química, Universidade de Aveiro, 3810-193 Aveiro, Portugal;

[‡]CIEPQPF, Departamento de Engenharia Química, FCTUC, Universidade de Coimbra, Rua Sílvio Lima, Pólo II – Pinhal de Marrocos, 3030-790 Coimbra, Portugal

[§]MATGAS Research Center (Carburos Metálicos/Air Products, CSIC, UAB), Campus UAB, 08193 Bellaterra, Barcelona, Spain.

[‡]Carburos Metálicos/Air ProductsGroup. C/Aragón, 300, 08009 Barcelona, Spain

*Corresponding author. Tel.: +351 234 401 507; Fax: + 351 234 370 084.

E-mail address: jcoutinho@ua.pt (J. A. P. Coutinho)

Table S. Bubble point data of the system CO₂ + [C₂mim][CH₃OHPO₂] and temperature dependent binary parameters (ζ) used in the soft-SAFT EoS.

x_{CO_2}	T (K)	p (MPa)	x_{CO_2}	T (K)	p (MPa)	x_{CO_2}	T (K)	p (MPa)
$m_{CO_2} = 0.423 \text{ mol}_{CO_2} \cdot \text{Kg}_{IL}^{-1}$			$m_{CO_2} = 0.795 \text{ mol}_{CO_2} \cdot \text{Kg}_{IL}^{-1}$			$m_{CO_2} = 1.861 \text{ mol}_{CO_2} \cdot \text{Kg}_{IL}^{-1}$		
0.080	293.21	1.16	0.141	293.29	1.88	0.277	293.16	3.42
	303.41	1.46		303.15	2.24		303.41	4.19
	313.45	1.76		313.46	2.45		313.52	5.08
	323.40	1.99		323.43	3.05		323.39	6.08
	333.29	2.31		333.46	3.56		333.32	7.21
	343.28	2.56		343.35	4.17		343.18	8.41
	353.50	2.85		353.31	4.75		353.33	9.80
	363.45	3.12		363.38	5.36		363.38	11.11
$m_{CO_2} = 2.607 \text{ mol}_{CO_2} \cdot \text{Kg}_{IL}^{-1}$			$m_{CO_2} = 3.353 \text{ mol}_{CO_2} \cdot \text{Kg}_{IL}^{-1}$			$m_{CO_2} = 3.997 \text{ mol}_{CO_2} \cdot \text{Kg}_{IL}^{-1}$		
0.350	293.17	5.21	0.409	293.28	6.45	0.452	293.32	11.00
	302.90	6.38		303.18	8.45		303.25	17.26
	313.23	7.54		313.18	11.48		313.29	23.51
	323.37	9.32		323.30	15.91		323.49	29.82
	333.23	11.27		333.24	20.47		333.53	34.67
	343.34	13.61		343.31	25.13		343.55	40.64
	353.32	16.20		353.46	29.45		353.46	45.99
	363.28	18.92		363.17	33.68		363.43	51.09
$m_{CO_2} = 4.932 \text{ mol}_{CO_2} \cdot \text{Kg}_{IL}^{-1}$							T_a^* (K)	ζ
0.504	293.18	31.91				293.23	1.022	
	303.26	40.79				303.22	1.021	
	313.41	49.64				313.36	1.020	
	323.31	58.70				323.38	1.017	
	333.35	66.69				333.36	1.014	
	343.31	73.43				343.33	1.010	
	353.34	80.89				353.39	1.005	
	363.32	87.65				363.34	1.000	

*Calculated average temperature.

Table S. Bubble point data of the system $N_2O + [C_2mim][CH_3OHPO_2]$ and temperature dependent binary parameters (ξ) used in the soft-SAFT EoS.

x_{N_2O}	T (K)	p (MPa)	x_{N_2O}	T (K)	p (MPa)	x_{N_2O}	T (K)	p (MPa)
$m_{N_2O} = 0.105$	$=0.569 \text{ mol}_{N_2O} \cdot \text{Kg}_{IL}^{-1}$		$m_{N_2O} = 0.137$	$=0.769 \text{ mol}_{N_2O} \cdot \text{Kg}_{IL}^{-1}$		$m_{N_2O} = 0.186$	$=1.110 \text{ mol}_{N_2O} \cdot \text{Kg}_{IL}^{-1}$	
	293.35	1.71		293.42	2.30		293.40	3.58
	303.37	2.13		303.30	2.88		303.22	4.39
	313.30	2.67		313.30	3.55		313.20	5.35
	323.32	3.22		323.13	4.23		323.34	6.42
	333.14	3.80		333.23	5.00		333.28	7.81
	343.25	4.45		343.25	5.71		343.23	9.04
	353.27	5.25		353.14	6.47		353.29	10.24
	363.40	5.75		363.39	7.32		363.47	11.47
$m_{N_2O} = 0.230$	$=1.450 \text{ mol}_{N_2O} \cdot \text{Kg}_{IL}^{-1}$		$m_{N_2O} = 0.249$	$=1.606 \text{ mol}_{N_2O} \cdot \text{Kg}_{IL}^{-1}$		$m_{N_2O} = 0.261$	$=1.716 \text{ mol}_{N_2O} \cdot \text{Kg}_{IL}^{-1}$	
	293.12	4.73		293.16	5.40		293.27	6.01
	303.26	5.93		303.41	6.88		303.19	9.31
	313.26	7.21		313.28	9.10		313.33	12.98
	323.28	8.76		323.23	11.93		323.14	15.95
	333.42	10.54		333.14	14.56		333.16	18.67
	343.18	12.36		343.10	17.08		343.25	21.30
	353.45	14.36		353.28	19.53		353.28	23.73
	363.37	16.23		363.29	21.74		363.24	25.87
$m_{N_2O} = 0.273$	$=1.819 \text{ mol}_{N_2O} \cdot \text{Kg}_{IL}^{-1}$		$m_{N_2O} = 0.281$	$=1.897 \text{ mol}_{N_2O} \cdot \text{Kg}_{IL}^{-1}$		$m_{N_2O} = 0.286$	$=1.946 \text{ mol}_{N_2O} \cdot \text{Kg}_{IL}^{-1}$	
	293.17	11.68		293.30	17.06		293.30	21.52
	303.22	15.15		303.26	19.78		303.11	24.18
	313.27	18.11		313.21	22.56		313.27	26.72
	323.30	20.98		323.16	25.15		323.25	29.25
	333.15	23.50		333.14	27.66		333.15	31.06
	343.22	25.95		343.19	30.05		343.16	33.07
	353.22	28.17		353.15	32.21		353.29	35.12
	363.25	30.19		363.11	34.13		363.14	36.99
$m_{N_2O} = 0.312$	$=2.196 \text{ mol}_{N_2O} \cdot \text{Kg}_{IL}^{-1}$						T_a^* (K)	ξ
	293.25	46.28						

303.31	48.66	293.27	0.9800
313.37	51.26	303.27	0.9820
323.49	52.47	313.28	0.9820
333.24	53.85	323.28	0.9805
343.29	54.85	333.21	0.9782
353.18	56.07	343.21	0.9753
363.40	56.75	353.26	0.9720
		363.31	0.9685

*Calculated average temperature.

Table S. Bubble point data of the system CH₄ + [C₂mim][CH₃OHPO₂] temperature dependent binary parameters (η) used in the soft-SAFT EoS.

x_{CH_4}	T (K)	P (MPa)	x_{CH_4}	T (K)	p (MPa)	x_{CH_4}	T (K)	p (MPa)
	$m_{CH_4} = 0.087 \text{ mol}_{CH_4} \cdot \text{Kg}_{IL}^{-1}$			$m_{CH_4} = 0.142 \text{ mol}_{CH_4} \cdot \text{Kg}_{IL}^{-1}$			$m_{CH_4} = 0.220 \text{ mol}_{CH_4} \cdot \text{Kg}_{IL}^{-1}$	
0.018	293.27	2.67	0.028	293.27	6.57	0.043	293.30	12.54
	303.25	2.93		303.32	6.84		303.38	12.76
	313.25	3.14		313.20	7.22		313.34	13.00
	323.29	3.36		323.22	7.55		323.31	13.12
	333.32	3.51		333.29	7.71		333.18	13.32
	343.25	3.66		343.08	7.94		343.19	13.42
	353.29	3.81		353.30	8.12		353.44	13.59
	363.31	3.86	363.21	8.23	363.43	13.78		
	$m_{CH_4} = 0.274 \text{ mol}_{CH_4} \cdot \text{Kg}_{IL}^{-1}$						T_a^* (K)	η
0.054	293.24	17.79					293.27	1.0505
	303.28	17.81					303.31	1.0457
	313.22	17.99					313.25	1.0435
	323.21	17.90					323.26	1.0430
	333.24	17.79					333.26	1.0438
	343.31	17.80					343.21	1.0455
	353.36	17.98					353.35	1.0475
	363.34	18.02				363.32	1.0500	

*Calculated average temperature.

Table S. Bubble point data of the system $N_2 + [C_2mim][CH_3OHPO_2]$ temperature dependent binary parameters (ξ) used in the soft-SAFT EoS.

x_{N_2}	T (K)	p (MPa)	x_{N_2}	T (K)	p (MPa)	x_{N_2}	T (K)	p (MPa)
$m_{N_2} = 0.084 \text{ mol}_{N_2} \cdot \text{Kg}_{IL}^{-1}$			$m_{N_2} = 0.107 \text{ mol}_{N_2} \cdot \text{Kg}_{IL}^{-1}$			$m_{N_2} = 0.132 \text{ mol}_{N_2} \cdot \text{Kg}_{IL}^{-1}$		
0.017	293.13	18.89	0.022	293.34	33.17	0.027	293.25	51.32
	303.13	16.99		303.50	31.12		303.14	46.93
	313.23	16.20		313.26	28.77		313.42	42.77
	323.48	15.67		323.16	27.54		323.34	39.80
	333.38	15.29		333.38	26.35		333.26	37.57
	343.46	15.14		343.38	25.10		343.22	35.79
	353.37	14.79		353.32	24.23		353.18	34.54
363.33	14.33	363.53	23.41	363.19	33.38			
$m_{N_2} = 0.155 \text{ mol}_{N_2} \cdot \text{Kg}_{IL}^{-1}$			$m_{N_2} = 0.177 \text{ mol}_{N_2} \cdot \text{Kg}_{IL}^{-1}$			$m_{N_2} = 0.200 \text{ mol}_{N_2} \cdot \text{Kg}_{IL}^{-1}$		
0.031	293.36	61.89	0.035	293.18	72.34	0.040	293.31	80.51
	303.37	55.20		303.32	64.21		303.24	72.11
	313.26	51.58		313.45	58.11		313.45	65.53
	323.30	48.12		323.35	53.55		323.18	60.50
	333.31	45.23		333.32	50.93		333.35	57.12
	343.23	42.72		343.21	47.78		343.32	53.37
	353.34	40.87		353.31	45.32		353.21	50.51
363.38	38.76	363.35	43.14	363.30	47.96			
$m_{N_2} = 0.222 \text{ mol}_{N_2} \cdot \text{Kg}_{IL}^{-1}$						T_a^* (K)		ξ
0.044	293.31	89.43				293.31	0.829	
	303.38	79.25				303.32	0.852	
	313.30	71.79				313.30	0.867	
	323.22	66.09				323.30	0.872	
	333.16	61.41				333.32	0.872	
	343.49	57.98				343.32	0.870	
	353.22	55.26				353.31	0.865	
363.28	52.18				363.33	0.859		

*Calculated average temperature.

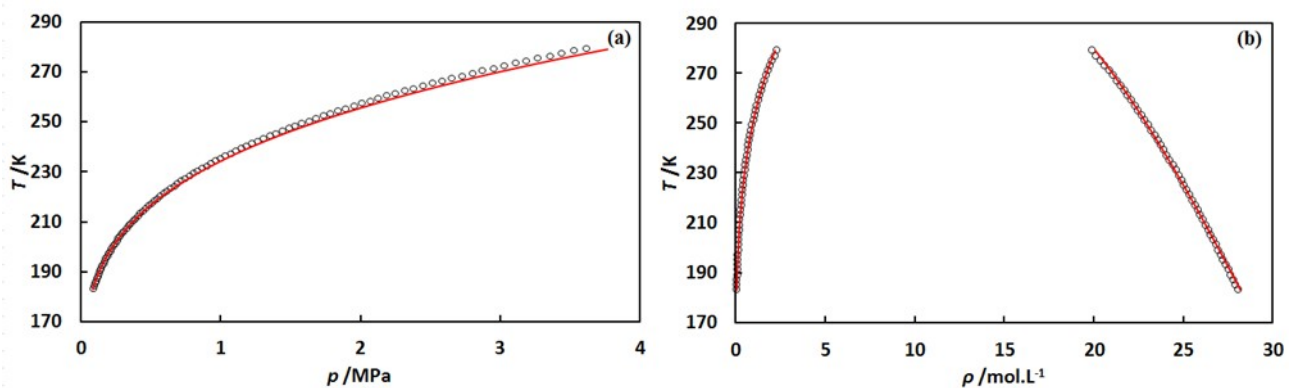


Figure S. (a) Temperature-vapor pressure and (b) temperature-density diagrams for N₂O. Symbols represent experimental data (Linstrom and Mallard, 2005) and the solid lines represent the soft-SAFT EoS fit.

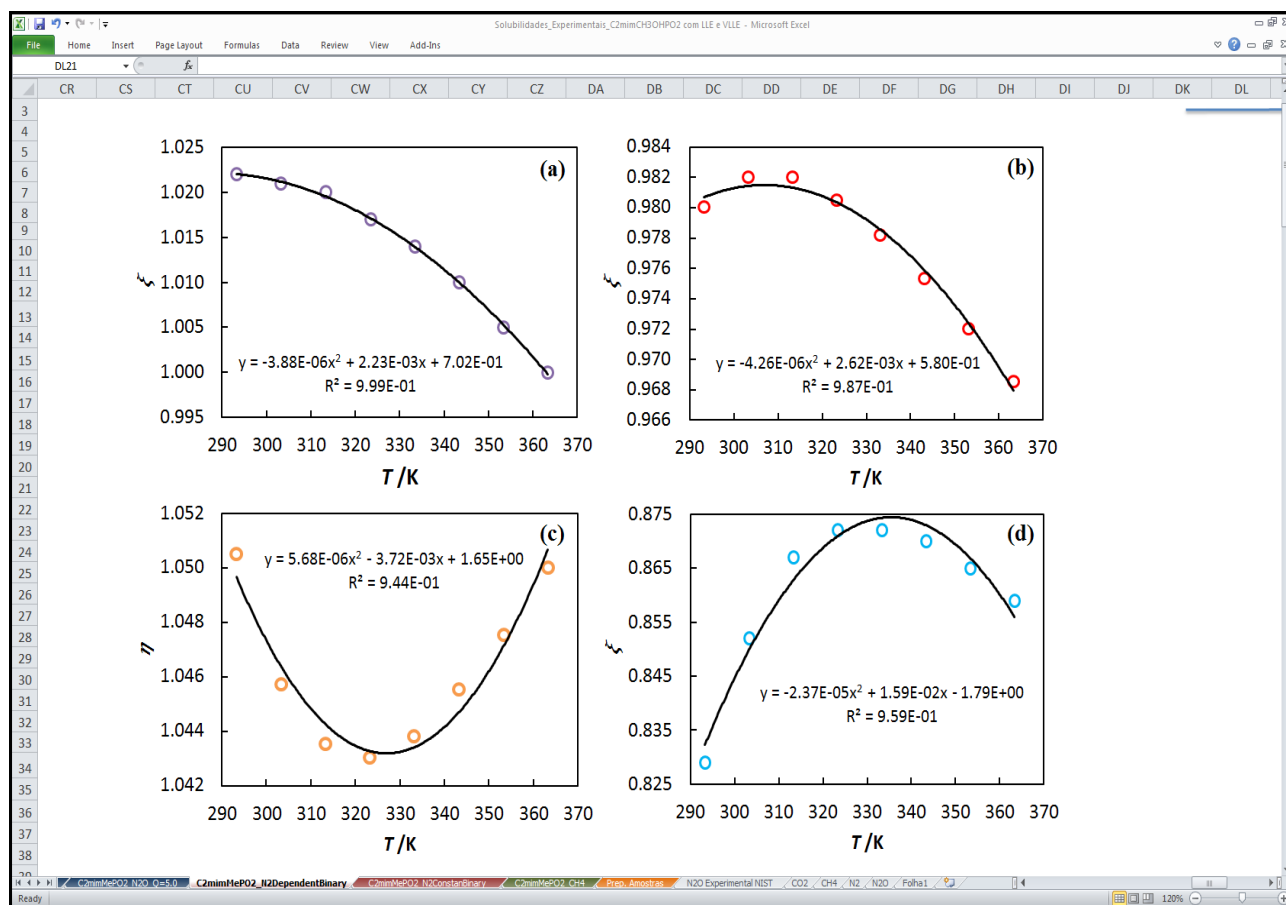


Figure S2. Soft-SAFT EoS binary parameter-temperature diagrams for the systems with the selected IL and the gases (a) CO₂, (b) N₂O, (c) CH₄ and (d) N₂. Solid lines represent the adjusted second order polynomial.

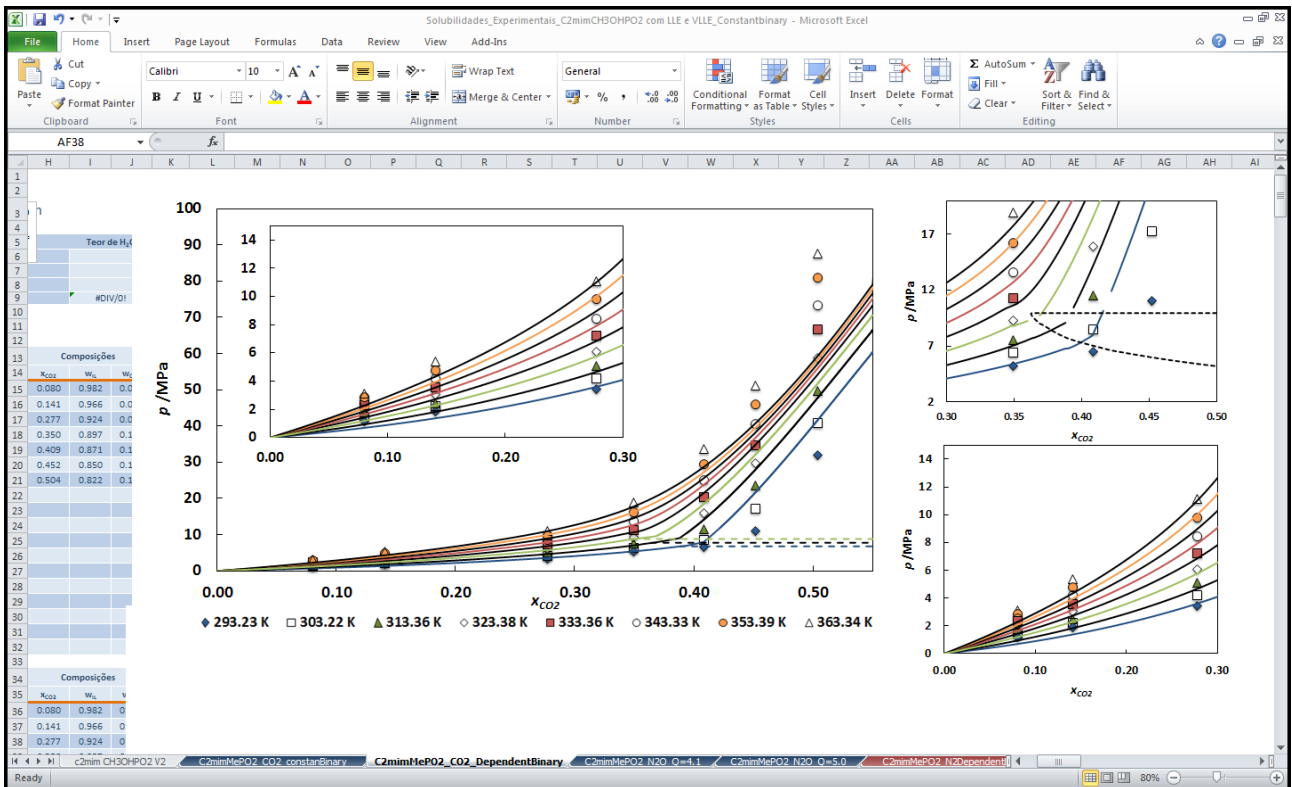


Figure S3. Pressure-composition diagram of the binary system $\text{CO}_2 + [\text{C}_2\text{mim}][\text{CH}_3\text{OHPO}_2]$. The solid lines represent the soft-SAFT EoS GLE predictions and the dashed lines the VLLC predictions, using one temperature independent binary parameter ($\xi = 1.0136$).