

*Supplementary Information*

# **Carbon Capture from Biogas by Deep Eutectic Solvents: A COSMO Study to Evaluate the Effect of Impurities on Solubility and Selectivity**

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Solubility	CO <sub>2</sub>			CH <sub>4</sub>			CO <sub>2</sub>			CH <sub>4</sub>			CO <sub>2</sub>			CH <sub>4</sub>		
Temp.	25 °C	25 °C	25 °C	25 °C	25 °C	25 °C	37 °C	37 °C	37 °C	37 °C	37 °C	37 °C	55 °C	55 °C	55 °C	55 °C	55 °C	55 °C
Mol %	1%	3%	5%	1%	3%	5%	1%	3%	5%	1%	3%	5%	1%	3%	5%	1%	3%	5%
H <sub>2</sub> O	1.00	0.98	0.96	0.99	0.98	0.96	1.00	0.98	0.96	0.99	0.98	0.96	1.00	0.98	0.96	0.99	0.98	0.96
CO <sub>2</sub>	-	-	-	1.00	1.00	0.99	-	-	-	1.00	1.00	1.00	-	-	-	1.00	1.00	1.00
CH <sub>4</sub>	1.00	1.00	1.00	-	-	-	1.00	1.00	1.00	-	-	-	1.00	1.00	1.01	-	-	-
Octa	1.00	1.02	1.07	1.00	1.04	1.09	1.00	1.03	1.08	1.01	1.05	1.11	1.01	1.04	1.10	1.01	1.06	1.13
Deca	1.00	1.04	1.10	1.01	1.06	1.14	1.01	1.05	1.12	1.01	1.07	1.16	1.01	1.06	1.14	1.02	1.09	1.19
H <sub>2</sub> S	1.00	1.01	1.01	0.99	0.98	0.97	1.00	1.01	1.01	1.00	0.99	0.98	1.00	1.01	1.01	1.00	0.99	0.98
NH <sub>3</sub>	1.01	1.02	1.04	1.00	1.01	1.02	1.01	1.02	1.04	1.00	1.01	1.01	1.01	1.02	1.04	1.00	1.01	1.01
N <sub>2</sub>	1.01	1.04	1.07	1.00	1.00	1.00	1.01	1.04	1.07	1.00	1.00	1.00	1.01	1.04	1.07	1.00	1.00	1.01
Acetone	1.01	1.03	1.05	1.01	1.02	1.04	1.01	1.03	1.05	1.01	1.02	1.04	1.01	1.03	1.05	1.01	1.02	1.04
SO <sub>2</sub>	1.00	1.00	1.00	1.00	0.99	0.98	1.00	1.00	1.00	1.00	0.99	0.99	1.00	1.00	1.00	1.00	0.99	0.99

**Table S1.** Normalized values for solubility of CO<sub>2</sub> and CH<sub>4</sub> at various mole percentages in ChCl: EG and at varying temperatures. The values are normalized to fresh solvent solubilities of respective CO<sub>2</sub> and CH<sub>4</sub>.

Solubility	CO <sub>2</sub>			CH <sub>4</sub>			CO <sub>2</sub>			CH <sub>4</sub>			CO <sub>2</sub>			CH <sub>4</sub>		
Temp.	25 °C	25 °C	25 °C	25 °C	25 °C	25 °C	37 °C	37 °C	37 °C	37 °C	37 °C	37 °C	55 °C	55 °C	55 °C	55 °C	55 °C	55 °C
Mol %	1%	3%	5%	1%	3%	5%	1%	3%	5%	1%	3%	5%	1%	3%	5%	1%	3%	5%
H <sub>2</sub> O	1.02	0.99	0.97	0.99	0.98	0.96	1.01	0.99	0.97	0.99	0.98	0.96	1.00	0.98	0.96	0.99	0.98	0.97
CO <sub>2</sub>	-	-	-	1.00	1.00	1.00	-	-	-	1.00	1.00	1.00	-	-	-	1.00	1.00	1.00
CH <sub>4</sub>	1.03	1.01	1.01	-	-	-	1.02	1.01	1.01	-	-	-	1.00	1.00	1.01	-	-	-
Octa	1.04	1.03	1.06	1.02	1.06	1.10	1.04	1.03	1.06	1.02	1.06	1.10	1.01	1.04	1.07	1.02	1.06	1.10
Deca	1.05	1.04	1.08	1.02	1.07	1.13	1.04	1.04	1.08	1.02	1.08	1.13	1.01	1.05	1.09	1.02	1.08	1.13
H <sub>2</sub> S	1.03	1.01	1.00	1.00	0.99	0.99	1.02	1.00	1.00	1.00	0.99	0.99	1.00	1.00	1.00	1.00	0.99	0.99
NH <sub>3</sub>	1.03	1.01	1.01	1.00	0.99	0.98	1.02	1.01	1.01	1.00	0.99	0.98	1.00	1.01	1.01	1.00	0.99	0.98
N <sub>2</sub>	1.04	1.02	1.05	1.00	1.00	1.01	1.03	1.02	1.05	1.00	1.00	1.01	1.01	1.02	1.04	1.00	1.00	1.01
Acetone	1.04	1.02	1.03	1.00	1.01	1.01	1.03	1.02	1.03	1.00	1.01	1.01	1.00	1.01	1.03	1.00	1.01	1.01
SO <sub>2</sub>	1.03	1.00	0.99	1.00	0.99	0.99	1.02	1.00	0.99	1.00	0.99	0.99	1.00	1.00	0.99	1.00	1.00	0.99

**Table S2.** Normalized values for solubility of CO<sub>2</sub> and CH<sub>4</sub> at various mole percentages in N4Cl: EG and at varying temperatures. The values are normalized to fresh solvent solubilities of respective CO<sub>2</sub> and CH<sub>4</sub>.

Solubility	CO <sub>2</sub>			CH <sub>4</sub>			CO <sub>2</sub>			CH <sub>4</sub>			CO <sub>2</sub>			CH <sub>4</sub>		
Temp.	25 °C	25 °C	25 °C	25 °C	25 °C	25 °C	37 °C	37 °C	37 °C	37 °C	37 °C	37 °C	55 °C	55 °C	55 °C	55 °C	55 °C	55 °C
Mol %	1%	3%	5%	1%	3%	5%	1%	3%	5%	1%	3%	5%	1%	3%	5%	1%	3%	5%
H <sub>2</sub> O	1.02	1.00	0.98	0.99	0.98	0.97	1.01	1.00	0.98	0.99	0.98	0.97	1.01	0.99	0.97	0.99	0.98	0.97
CO <sub>2</sub>	-	-	-	1.00	0.99	0.99	-	-	-	1.00	0.99	0.99	-	-	-	1.00	0.99	0.99
CH <sub>4</sub>	1.03	1.01	1.00	-	-	-	1.02	1.00	1.00	-	-	-	1.01	1.00	0.99	-	-	-
Octa	1.03	1.01	1.02	1.01	1.02	1.04	1.03	1.01	1.02	1.01	1.02	1.04	1.02	1.01	1.02	1.01	1.02	1.04
Deca	1.04	1.01	1.02	1.01	1.03	1.05	1.03	1.01	1.02	1.01	1.03	1.05	1.02	1.01	1.03	1.01	1.03	1.05
H <sub>2</sub> S	1.03	1.01	1.00	1.00	0.99	0.98	1.02	1.00	0.99	1.00	0.99	0.98	1.01	1.00	0.99	1.00	0.99	0.98
NH <sub>3</sub>	1.03	1.01	1.00	1.00	0.98	0.97	1.02	1.00	1.00	1.00	0.98	0.97	1.01	1.00	1.00	1.00	0.98	0.97
N <sub>2</sub>	1.03	1.01	1.02	1.00	1.00	0.99	1.02	1.01	1.01	1.00	1.00	0.99	1.02	1.01	1.01	1.00	1.00	0.99
Acetone	1.03	1.01	1.01	1.00	0.99	0.99	1.02	1.01	1.00	1.00	0.99	0.99	1.01	1.00	1.00	1.00	0.99	0.99
SO <sub>2</sub>	1.02	1.00	0.99	1.00	0.99	0.98	1.02	1.00	0.99	1.00	0.99	0.98	1.01	0.99	0.98	1.00	0.99	0.98

**Table S3.** Normalized values for solubility of CO<sub>2</sub> and CH<sub>4</sub> at various mole percentages in N4Br: DA and at varying temperatures. The values are normalized to fresh solvent solubilities of respective CO<sub>2</sub> and CH<sub>4</sub>.

Solubility	CO <sub>2</sub>			CH <sub>4</sub>			CO <sub>2</sub>			CH <sub>4</sub>			CO <sub>2</sub>			CH <sub>4</sub>		
Temp.	25 °C	25 °C	25 °C	25 °C	25 °C	25 °C	37 °C	37 °C	37 °C	37 °C	37 °C	37 °C	55 °C	55 °C	55 °C	55 °C	55 °C	55 °C
Mol %	1%	3%	5%	1%	3%	5%	1%	3%	5%	1%	3%	5%	1%	3%	5%	1%	3%	5%
H <sub>2</sub> O	1.03	1.02	0.99	1.00	0.98	0.97	1.02	1.00	0.98	1.00	0.98	0.97	1.01	0.99	0.98	1.00	0.98	0.97
CO <sub>2</sub>	-	-	-	1.00	0.99	0.99	-	-	-	1.00	0.99	0.99	-	-	-	1.00	0.99	0.99
CH <sub>4</sub>	1.04	1.03	1.00	-	-	-	1.03	1.00	1.00	-	-	-	1.02	1.00	0.99	-	-	-
Octa	1.04	1.04	1.01	1.00	1.01	1.02	1.03	1.01	1.01	1.00	1.01	1.02	1.02	1.01	1.01	1.00	1.01	1.02
Deca	1.04	1.05	1.02	1.00	1.02	1.03	1.03	1.01	1.02	1.00	1.02	1.03	1.02	1.01	1.02	1.00	1.02	1.03
H <sub>2</sub> S	1.03	1.03	1.00	1.00	0.99	0.98	1.02	1.00	0.99	1.00	0.99	0.98	1.01	1.00	0.99	1.00	0.99	0.98
NH <sub>3</sub>	1.04	1.03	1.01	1.00	0.99	0.97	1.03	1.01	1.00	1.00	0.99	0.97	1.02	1.00	1.00	1.00	0.99	0.98
N <sub>2</sub>	1.04	1.04	1.01	1.00	0.99	0.99	1.03	1.01	1.01	1.00	0.99	0.99	1.02	1.01	1.01	1.00	0.99	0.99
Acetone	1.04	1.04	1.01	1.00	0.99	0.98	1.03	1.01	1.00	1.00	0.99	0.98	1.02	1.00	1.00	1.00	0.99	0.98
SO <sub>2</sub>	1.03	1.02	1.00	1.00	0.99	0.98	1.02	1.00	0.99	1.00	0.99	0.98	1.01	1.00	0.99	1.00	0.99	0.98

**Table S4.** Normalized values for solubility of CO<sub>2</sub> and CH<sub>4</sub> at various mole percentages in N8Br: DA and at varying temperatures. The values are normalized to fresh solvent solubilities of respective CO<sub>2</sub> and CH<sub>4</sub>.