Supplementary Information for:

Soil sorption of two nitramines derived from amine-based CO₂ capture

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Table of contents:

- A. Nitramine standards
- **B.** Soil samples
- C. Characterization of soil samples and aqueous soil extracts
- D. Soil characteristics
- E. Correlation analysis
- F. Sorption isotherms

A. Nitramine standards

Table A1: Abbreviation, name, and CAS number for MEA- and DMA-nitramine, in addition to the precursor molecule for MEA-nitramine (3-nitro-oxazolidin-2-one).

Abbreviation	Name	CAS no.
MEA-nitramine	N-nitroethanolamine	74386-82-6
DMA-nitramine	N-nitrodimethylamine	4164-28-7
Precursor for MEA-nitramine	3-nitro-oxazolidin-2-one	85430-60-0

B. Soil samples



Figure B1: Sampling sites in relation to the Technology Centre Mongstad (left) and the five sampling plots (right).

Sample ID	Depth (cm)	Altitude (m.a.s.l)	Slope (°,OR)	Vegetation	Remark	Coordinates
PZI-O	0-2	289	40-50, NW	Birch, sphagnum moss, sedges, common juniper, cranberry heath	Blocky soil	60°55′17" N 05°10′46"
PZs-O	0-5	211	40-50,	Planted spruce wood		60°55′07″ N
PZs-A	5-30		W-NW		Stony, blocky	05°10′35″
PZs-Bhs	30-50				Stony	
PZg-B	15-25	125	0, N/A	Grass, common juniper, moss	Next to riverbed	60°55'17" N 05°10'22"
HSf-e	0-70	61	0, N/A	Grass, previously	Boggy pasture	60°55′47″ N
HSf-a	80-			cultivated		05°10′13′′
	120					
HSh-i	10-60	51	0, N/A	Bog	sphagnum moss	60°55′44′′ N
					on top	05°9'58''

Table B1: Origin- and sampling details of the soil samples.

C. Characterization of soil samples and aqueous soil extracts

The soil samples were air dried and sieved (2.0 mm) according to ISO 11464 (2006), and stored in the dark at room temperature until analysis. The dry mass of the soil samples was determined gravimetrically by drying each sample at 105 °C for 6 h according to ISO 11465 (1993). The content of SOM was determined gravimetrically using the method of loss on ignition according to Krogstad (1992) by igniting the samples at 550 °C for 3 h. Resulting mass loss was attributed to the combustion of organic matter. Conversion from SOM to soil organic carbon (SOC) was calculated using a factor of 1.86 for soils rich in organic matter (SOM > 30 %, w/w) and 1.72 for mineral soils (SOM < 30 %) (Delle Site, 2001 and references therein). The soil pH was determined according to ISO 10390 (2005), in 0.01 M CaCl₂, and using an Orion Research Expandable Ion Analyser EA 920 with a ROSS pH-electrode (Thermo Scientific, Waltham, MA, USA). Two different fractions of aluminium (AI) and iron (Fe), consisting of dissolved amorphous- and hydrous oxides ("active") and organically bound ("organic"), were extracted from the soils using the methods described by ISRIC (2002). "Active" Al and Fe were extracted using a complexing acid ammonium oxalate solution, while the organically bound Al and Fe was extracted using a sodium pyrophosphate solution. Quantification of resulting Al- and Fe-pools was performed using an inductively coupled plasma-atomic emission spectrometer (ICP-OES, Varian Vista) with axial view and equipped with a charge coupled device detection system. Additionally for the mineral soil samples (SOM < 30 %, w/w) both the particle size distribution (according to ISO 11277 (2009)) and the mineralogy (X-ray diffraction) was determined, the latter using a D8 Discover powder diffractometer (Bruker AXS, Karlsruhe, Germany).

The aqueous soil extracts produced from the soil sorption experiment (section 2.4) were analysed for the following parameters: pH (instrumentation described above), conductivity using a FG3 portable conductivity meter (Mettler-Toledo, Greifensee, Switzerland), and concentration of dissolved organic carbon (DOC) was measured using the method of non-purgeable organic carbon on a TOC-V_{CPH} Total Organic Carbon Analyzer (Shimadzu, Kyoto, Japan). Qualitative characterization of the leached dissolved organic matter (DOM) was performed by measuring absorbency in the UV-Vis range from 200 to 600 nm (UV-1800 UV-Vis spectrophotometer, Schimadzu, Kyoto, Japan).

D. Soil characteristics

Sample ID	Dry matter
	content (%, w/w)
PZI-O	95.8
PZs-O	92.2
PZs-A	96.2
PZs-Bhs	96.2
PZg-B	98.9
HSf-e	91.0
HSf-a	90.2
HSh-i	91.2

Table D1: Dry matter content (%, w/w) of the soil samples.

Sample	Sand % (w/w)	Silt % (w/w)	Clay % (w/w)	Total % (w/w)	Texture
PZs-A	70	21	10	101	Sandy loam
PZs-Bhs	57	34	9	100	Sandy loam
PZg-B	72	22	5	99	Sandy loam

Table D2: Particle size distribution (PDS) of the mineral soil samples (Eurofins).

Table D3: Main mineral composition of the soil samples (XRD).

Sample	Quartz (%, w/w)	Albite (%, w/w)	Oligoclase (%, w/w)	Labradorite (%, w/w)	Bytownite (%, w/w)	Other specified (%, w/w)
PZI-O	30	18	38		13	
PZs-O	34	12	23	31		
PZs-A	22		51	18		10 Kalifersite
PZs-Bhs	39	41	20			
PZg-B	37	11	50			1 Kalifersite 1 Sklodowskite 0.3 Algodonite
HSf-e	25		75			
HSf-a	31		69			
HSh-i	23	54	22			

Al- and Fe- hydroxides



Figure D1: Amount of "Active" (light coloured) and organic (dark coloured) aluminium (solid) and iron (stripe) extracted from the soils. Error bars illustrate one standard deviation from measurement replicates (n=3).

E. Correlation analysis

A rather strong correlation between MEA- and DMA-nitramine soil sorption and the conductivity measured in the aqueous soil extracts is evident (r = 0.916, 0.669, C \ge 98 %, 95 %). This is however believed to be a confounding factor since the DOM leached from the soil largely contributes to the measured conductivity. Only a weak correlation is found between soil pH /H⁺ and nitramine soil sorption (C < 90 %). This is likely due to the narrow range in pH values displayed by these soils.

Characterization parameter	K _d (L k	g soil-1)	K _{oc} (L kg OC ⁻¹)		
	MEA-NO ₂	DMA-NO ₂	MEA-NO ₂	DMA-NO ₂	
OM (%, w/w)	0.72*	0.95***	-0.27	0.53	
pH (CaCl ₂)	-0.65	-0.23	-0.55	0.17	
H ⁺ (CaCl ₂)	0.70	0.16	0.65	-0.17	
Cond (µS cm ⁻¹)	0.92***	0.67	0.22	0.17	
DOC (g kg ⁻¹)	0.85**	0.54	0.44	-0.021	
DOC:SOC (g kg ⁻¹)	-0.20	-0.52	0.44	-0.63	
Al-Org (mol/kg soil)	-0.38	0.036	-0.72*	0.020	
Fe.Org (mol/kg soil)	-0.58	-0.35	-0.39	0.085	
Al.Active (mol/kg soil)	-0.67	-0.52	-0.44	-0.55	
Fe.Active (mol/kg soil)	-0.56	-0.28	-0.54	-0.062	
Abs 254nm	0.93***	0.41	0.47	-0.089	
Abs 400nm	0.95***	0.55	0.40	0.11	
sUVa (Abs _{254nm} /DOC*100)	0.78**	0.46	0.36	0.071	
sVISa (Abs _{400nm} /DOC*1000)	0.75*	0.60	0.26	0.34	
SAR (Abs _{254nm} /Abs _{400nm})	-0.42	-0.60	-0.11	-0.85***	
Quartz.low (%, w/w)	-0.43	-0.48	0.23	-0.17	
Albite (%, w/w)	0.001	0.11	0.093	0.40	
Oligoclase (%, w/w)	0.27	0.37	-0.10	0.15	

Table E1: Values of r² describing the correlation between the soil water distribution coefficient (K_d)- and the organic carbon normalized soil-water distribution coefficient (K_{oc}) of MEA- and DMA-nitramine and soil characteristics.

*90 % (p < 0.05) confidence level

**95 % (p < 0.025) confidence level

*** ≥ 98 % (0.01) confidence level

	K _d (L k	g soil ⁻¹)	K _{oc} (L kg OC ⁻¹)	
Characterization parameter	MEA-NO ₂	DMA-NO ₂	MEA-NO ₂	DMA-NO ₂
OM (%, w/w)	0.043	0.0004	0.52	0.18
pH (CaCl ₂)	0.081	0.58	0.16	0.69
H^+ (CaCl ₂)	0.067	0.70	0.083	0.69
Cond (µS cm ⁻¹)	0.0014	0.070	0.61	0.69
DOC (g kg ⁻¹)	0.00041	0.16	0.70	0.96
DOC:SOC (g kg ⁻¹)	0.54	0.19	0.30	0.091
Al-Org (mol/kg soil)	0.35	0.93	0.043	0.96
Fe.Org (mol/kg soil)	0.13	0.40	0.34	0.84
Al.Active (mol/kg soil)	0.071	0.19	0.27	0.16
Fe.Active (mol/kg soil)	0.15	0.50	0.17	0.88
Abs 254nm	0.00071	0.32	0.24	0.83
Abs 400nm	0.00033	0.16	0.32	0.79
sUVa (Abs _{254nm} /DOC*100)	0.023	0.26	0.39	0.87
sVISa (Abs _{400nm} /DOC*1000)	0.032	0.12	0.54	0.42
SAR (Abs _{254nm} /Abs _{400nm})	0.30	0.12	0.79	0.0082
Humic acid:Fulvic acid	0.97	0.81	0.41	0.14
Quartz.low (%, w/w)	0.29	0.23	0.58	0.68
Albite (%, w/w)	1.0	0.80	0.83	0.32
Olgioclase (%, w/w)	0.51	0.37	0.81	0.73

Table E2: Values of p describing the significance of the correlation between the soil water distribution coefficient (K_d) and the organic carbon normalized soil-water distribution coefficient (K_{oc}) of MEA- and DMA-nitramine and soil characteristics.



Figure E1: Correlation matrix for the MEA-nitramine soil-water distribution coefficient (K_d) and selected soil descriptors. The distribution of each variable is shown on the diagonal. Above the diagonal, Pearson's correlation coefficient (r) is provided with significance levels (p-values) indicated using stars (*** \geq 0.01, ** \geq 0.025, * \geq 0.05, $\cdot \geq$ 0.1). On the bottom of the diagonal the bivariate scatter plots with a fitted line are displayed.



Figure E2: Correlation matrix for the DMA-nitramine soil-water distribution coefficient (K_d) and selected soil descriptors. The distribution of each variable is shown on the diagonal. Above the diagonal, Pearson's correlation coefficient (r) is provided with significance levels (p-values) indicated using stars (*** \geq 0.01, ** \geq 0.025, * \geq 0.05, $\cdot \geq$ 0.1). On the bottom of the diagonal the bivariate scatter plots with a fitted line are displayed.

MEA-nitramine							
$K_{d} = OM + (Abs_{254nm})^{2}$							
Multiple r ²	0.938						
Adjusted r ²	0.914						
p-value	0.000942						
F-statistic	0.381 on 2 and	15					
_	DF						
Coefficients:							
Parameter	Estimate	Std. Error	T value	Pr (> t)	_		
Intercept	0.0591	0.110	0.536	0.615			
OM	0.00757	0.002530	2.99	0.0304			
(Abs456nm)^2	0.483	0.0828	5.83	0.00211			
Residuals:					-		
1	2	3	4	5	6	7	8
-0.0695	0.0831	-0.0229	-0.104	0.0908	0.00451	0.265	-0.247
Residual std. error	0.1805 on 5						
	DF						

Table E3: Multiple linear regression analysis for MEA-nitramine soil sorption, K_d = OM + Abs_{254nm}²

Table E4: Multiple linear regression analysis for DMA-nitramine soil sorption, K_d = OM

DMA-ni	tramine			
K _d =	OM			
Multiple r ²	0.894			
Adjusted r ²	0.876			
p-value	0.000387			
F-statistic	50.6			
Coefficients:				
Parameter	Estimate	Std. Error	T value	Pr (> t)
Intercept	-0.250	0.198	-1.26	0.254
OM	0.0292	0.00411	7.12	0.000387
Residuals:				
Min	Q1	Median	Q3	Max
-0.4720	-0.230	0.140	0.226	0.302
Residual std. error	0.3319 on 6 DF			

F. Sorption isotherms

 Table F1: Fitting parameters obtained from linear and Freundlich models for soil sorption isotherms of MEA-nitramine.

 The uncertainty equals to the standard error of the estimates.

	Linea	r	Freundlich			
Sample ID	K _d	r ²	K _F	n	r ²	
	(L kg ⁻¹)		(mg ¹⁻ⁿ L ⁿ kg ⁻¹)			
PZI-O	1.8 ± 0.1	0.93	0.4 ± 0.3	2.1 ± 0.6	0.77	
PZs-O	0.41 ± 0.1	0.45	1.2 ± 1	0.31 ± 0.2	0.41	
HSf-e	0.8 ± 0.1	0.76	0.8 ± 2	0.7 ± 0.4	0.36	
HSh-i	0.9 ± 0.2	0.60	1.3 ± 2	0.5 ± 0.3	0.44	
HSf-a	0.99 ± 0.06	0.96	1.5 ± 0.2	0.69 ± 0.06	0.97	

 Table F2: Fitting parameters obtained from linear and Freundlich models for soil sorption isotherms of DMA-nitramine.

 The uncertainty equals to the standard error of the estimates.

	Linea	r	Freundlich		
Sample ID	K _d r ²		K _F	n	r ²
	(L kg⁻¹)		(mg ¹⁻ⁿ L ⁿ kg ⁻¹)		
PZI-O	0.49 ± 0.1	0.24	0.8 ± 0.8	0.7 ± 0.2	0.79
PZs-O	0.29 ± 0.1	0.32	0.4 ± 0.1	0.9 ± 0.3	0.69
HSf-e	1.15 ± 0.03	0.99	1.2 ± 0.8	1.02 ± 0.09	0.97
HSh-i	2.0 ± 0.3	0.75	1.6 ± 0.5	1.2 ± 0.1	0.95
HSf-a	2.2 ±0.1	0.96	2.5 ± 0.3	0.8 ± 0.1	0.94

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