

Soil chemical data

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Introduction

In this data sheet all measured soil chemical variables per soil plot depth increment, soil pit horizon and bioplot are shown. These data entail the sample id, plot id, site id, pH, CEC, exchangeable cations, total reserve in base cations, sequentially-extracted pedogenic oxide concentrations, total elemental concentrations by aqua regia digestion and measurement by inductively-coupled plasma optical emission spectroscopy (ICP-OES) and total elemental concentrations by X-ray fluorescence (XRF) measurement.

Table 1. General information

project_name	ETH+ Arctic Greening
creation_date	2025-01-15
last_modification_date	2025-03-05
sampling_period	2022-07-09 – 2023-08-09
creator	Annina Maier
contact_1	annina.maier@usys.ethz.ch
contact_2	sdoetterl@usys.ethz.ch
number_samples	497
processing_status	ongoing
upload_status	ongoing

Table 2. Variable overview

upload_status	structured	
variable	explanation	unit
plot_id	plot_id of a respective observation	-
sample_id	sample_id of a respective observation	-
pH_CaCl2	pH of the bulk soil measured with CaCl ₂	-
pH_CaCl2_predicted	Indication if the pH value in the pH_CaCl2 column was observed or predicted using a DRIFT spectroscopy calibrated model. For details see soil spectroscopy metadata	-
CECeff_BaCl2	Effective cation exchange capacity of the bulk soil measured in BaCl ₂ . Calculated as $\sum$ Ca, K, Mg, Na exchangeable cations	cmol _c kg ⁻¹
CECeff_BaCl2_predicted	Indication if the effective cation exchange capacity value in the CECeff column was observed or predicted using a DRIFT spectroscopy	-

	calibrated model. For details see soil spectroscopy metadata	
Al_BaCl2, Ca_BaCl2, Fe_BaCl2, K_BaCl2, Mg_BaCl2, Mn_BaCl2, Na_BaCl2	Exchangable Al, Ca, Fe, K, Mg, Mn, Na cations measured in BaCl ₂	cmol _c kg ⁻¹
Al_PP, Fe_PP, Mn_PP, Si_PP	Pyrosphosphate-extractable Al, Fe, Mn and Si pedogenic oxides	g kg ⁻¹
Al_AO, Fe_AO, Mn_AO, Si_AO	Ammonium oxalate-extractable Al, Fe, Mn and Si pedogenic oxides	g kg ⁻¹
Mn_AO_predicted	Indication if the ammonium oxalate-extractable Mn pedogenic oxides in the Mn_AO column was observed or predicted using a DRIFT spectroscopy calibrated model. For details see soil spectroscopy metadata	-
Al_DCB, Fe_DCB, Mn_DCB, Si_DCB	Dithionite citrate bicarbonate-extractable Al, Fe, Mn and Si pedogenic oxides	g kg ⁻¹
Fe_DCB_predicted	Indication if dithionite citrate bicarbonate-extractable Fe pedogenic oxides in the Fe_DCB column was observed or predicted using a DRIFT spectroscopy calibrated model. For details see soil spectroscopy metadata	-
Al_AR, Ca_AR, Fe_AR, K_AR, Mg_AR, Mn_AR, Na_AR, Si_AR, P_AR	Total elemental concentrations of Al, Ca, Fe, K, Mg, Mn, Na, Si, P, by aqua regia digestion and measurement by ICP-OES	g kg ⁻¹
TRB	Total reserve in base cations, i.e. sum of total Ca, Na, K and Mg	g kg ⁻¹
Al_XRF, Si_XRF, P_XRF, S_XRF, Cl_XRF, K_XRF, Ca_XRF, Ti_XRF, Cr_XRF, Mn_XRF, Fe_XRF, Co_XRF, Ni_XRF, Cu_XRF, Zn_XRF, As_XRF, Se_XRF, Sr_XRF, Zr_XRF, Cd_XRF	Total elemental concentrations of Al, Si, P, S, Cl, K, Ca, Ti, Cr, Mn, Fe, Co, Ni, Cu, Zn, As, Se, Sr, Zr, Cd, by XRF	µg g ⁻¹
Al_XRF_predicted, Ca_XRF_predicted, Fe_XRF_predicted, K_XRF_predicted, Mg_XRF_predicted, Si_XRF_predicted	Indication if the total elemental concentrations in the Al, Si, P, S, Cl, K, Ca, Ti, Cr, Mn, Fe, Co, Ni, Cu, Zn, As, Se, Sr, Zr, Cd-XRF column was observed or predicted using a DRIFT spectroscopy calibrated model. For details see soil spectroscopy metadata	-

Methods

Sample processing

pH analyses were carried out with 30 °C dried and sieved soil samples (< 2 mm). Effective cation exchange capacity, sequential extraction of pedogenic oxides and total elemental

composition analyses (Aqua regia + ICP-OES, XRF) were carried out with 30 °C dried and powder-milled (Mixer Mill MM 200, Retsch GmbH Haan, Germany) soil samples.

Sample analysis

pH

For the pH measurement, 15 ml of 0.01 M CaCl_2 was added to 3 g of soil sample in a 50 ml falcon tube. The samples were shaken horizontally for 10 min at high intensity then left to stand for 24 h until measurement using a pH meter (Metrohm 713).

Effective cation exchange capacity

Effective cation exchange capacity (CEC_{eff}) and the amount of exchangeable cations (Ca, Mg, K, Na, Al, Fe, Mn) were determined according to Hendershot (1986) using BaCl_2 . In brief, 20 ml of 0.1M BaCl_2 were added to 3 g of soil in a 50 ml centrifuge tube. These samples were then placed on a horizontal shaker for 2 h at a setting of 150 shakes per minute. After, they were centrifuged at 2500 rpm for 10 min and filtered (42 μm) into 50 ml tubes. Extracts were then stored at room temperature before measurement. Shortly before measurement on the Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES) (5100 ICP-OES, Agilent Technologies, Santa Clara, CA, United States), samples were diluted 1:10 with MQ and 0.1 ml of internal standard (in HNO_3 , 65 %).

Sequential extraction of pedogenic oxides

Fe, Al and Mn oxy(hydr-)oxides were extracted sequentially in the following sequence: first sodium pyrophosphate (PP) (Bascomb, 1968), second ammonium oxalate (AO) (Dahlgren, 1994), and lastly with dithionite-citrate-bicarbonate solutions (Mehra, 1958). The extraction procedure is based on duplicate extractions, hence, each sample was extracted twice in the form of two subsamples which were merged for final measurement with ICP-OES (5100 ICP-OES, Agilent Technologies, Santa Clara, CA, United States). For this sequential extraction the following reagents were prepared: i) sodium-pyrophosphate solution, ii) ammonium oxalate solution

The sodium-pyrophosphate solution was made by adding 44.61 g of 0.1 M $\text{Na}_4\text{P}_2\text{O}_7 \times 10 \text{ H}_2\text{O}$ and 71.02 g of 0.5 M Na_2SO_4 to 1 L MQ (should have a pH of 10). The ammonium oxalate solution was made by mixing 0.2 M ammonium oxalate and 0.2 M oxalic acid dihydrate in a ratio of 1:31:1. The pH of this mixture was then adjusted to 3.

For sodium-pyrophosphate- (PP) extractable pedogenic oxides, 0.25 g of 30 °C dried and milled bulk soil was weighed-in to a 15 ml centrifuge tube. To this, 10 ml of sodium-pyrophosphate solution was added, and the solution was vortexed. The centrifuge tubes were then closed and placed on a horizontal shaker to shake overnight (16 h). Then the samples were centrifuged at 3000 rpm (~1700 g) at 20 °C for 10 min. The supernatants of two corresponding samples were then transferred through a filter (Whatman 41) into a new 50 ml centrifuge tube. The remaining soil contained in the centrifuge tube was kept for the next extraction step. The new 50 ml centrifuge tube was then filled to 50 ml with MQ. These extracts were stored at 4° C prior to measurement on ICP-OES.

For the ammonium-oxalate- (AO) extractable pedogenic oxides 10 ml of ammonium oxalate solution was added to the soil samples in the 15 ml centrifuge tubes. After vortexing and ultrasonication the samples, they were placed into a dark box and put on a horizontal shaker to shake for 2 h. Then the samples were centrifuged at 3000 rpm (~1700 g) at 20 °C for 10

min. The supernatants of two corresponding samples were then transferred through a filter (Whatman 41) into a new 50 ml centrifuge tube, which contained 0.5 ml 0.02 M KCl. The remaining soil contained in the centrifuge tube was kept for the next extraction step. The new 50 ml centrifuge tube was then filled to 50 ml with MQ. These extracts were stored at 4° C prior to measurement on ICP-OES.

For the dithionite-citrate-bicarbonate- (DCB) extractable pedogenic oxides 10 ml of 0.3 M sodium citrate solution was added to the soil samples in the 15 ml centrifuge tubes. On top of this 1.25 ml of 1 M NaHCO₃ were added and then the samples were vortexed. The samples were then placed in a pre-heated water (70 – 75 °C) bath filled with MQ and shaken regularly by hand. The samples were then removed from the water bath, had 0.25 g sodium dithionite added to them and were then shaken rigorously. They were then placed back into the water bath for 15 min, whilst being shaken again regularly during this time. This procedure was repeated until samples looked grey-coloured, after which samples were left to cool outside the bath for 5-10 min. The samples then were centrifuged at 4000 rpm for 10 min. The supernatants of two corresponding samples were then transferred through a filter (Whatman 41) into a new 50 ml centrifuge tube, which contained 0.5 ml 0.02 M KCl. 5 ml of MQ water were added to the centrifuge tubes containing the remaining soil pellet and were then vortexed. The samples were then centrifuged again at 3000 rpm for 10 min and again the supernatants of two corresponding samples were transferred through a filter (Whatman 41) into the 50 ml centrifuge tube containing the previous supernatant solutions. This procedure was repeated once more. Then, 2.5 ml of magnesium sulfate was added to the soil pellets and they were vortexed and ultrasonicated. The samples were centrifuged at 3000 rpm for 10 min and again the supernatants of two corresponding samples were transferred through a filter (Whatman 41) into the 50 ml centrifuge tube containing the previous supernatant solutions. These extracts were stored at 4° C prior to measurement on ICP-OES.

Total elemental composition and total reserve in base cations (TRB)

Total elemental composition of the soil and parent material samples was determined by applying two techniques: X-ray fluorescence (XRF) spectrometry for the heavier elements Si, Ti and Zr, and inductively coupled plasma optical emission spectrometry (ICP-OES) (5100 ICP-OES, Agilent Technologies, Santa Clara, CA, United States) for the elements Na, K, Ca, Mg, Al, Fe and Mn.

For the total elemental composition analysis by ICP-OES an aqua regia digestion was conducted. Hereby, 1 g of 30 °C dried and milled bulk soil material was weighed into a DigiPrep tube. To this 2 ml of MQ, then 2 ml of HNO₃ (65%) and lastly 6 ml of HCl (37%) were added. The tubes were covered with watchglasses and placed into the extraction block for a 150 min. During this time the block was heated up from room temperature until 120 °C. After, the samples were removed from the extraction block and cooled under a fume hood. The tubes were then filled up until 50 ml with MQ and transferred through a filter (Whatman 41) into new 50 ml Falcon tubes. These extracts were stored at room temperature prior to measurement on ICP-OES. Total reserve in base cations was calculated by summing up total Ca, Na, K and Mg concentrations (ΣCa_AR , Na_AR , K_AR , Mg_AR).

For the total elemental composition analysis by XRF 4 g of 30 °C dried and milled bulk soil was mixed with 0.9 g Licowax for 8 min at 24 shakes per second using a ball mill (Retsch MM200). The resulting mix was then pressed to a pellet using a press (Specac Portmann Instruments AG). These pellets were then measured on XRF (AMATEK Spectro XEPOS). Note

that XRF results are reported as elemental concentrations (wt. %), not oxide equivalents. Oxygen was not measured, which accounts for the total elemental sum being significantly below 100%.

References

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