Isotope geochemical dataset on subsoil management experiments at Campus Klein-Altendorf (https://doi.org/10.5880/fidgeo.2022.003)

Uhlig, David

Institute of Bio- and Geosciences (IBG-3) Agrosphere, Forschungszentrum Jülich GmbH, Wilhelm-Johnen Straße, 52425 Jülich, Germany

1. Licence

2. Citation

When using the data please cite:

Uhlig, David (2022): Isotope geochemical dataset on subsoil management experiments at Campus Klein-Altendorf. GFZ Data Services. https://doi.org/10.5880/fidgeo.2022.003

The data are supplementary material to:
Uhlig, D., Wu, B., Berns, A.E., Amelung, W. (2022): Magnesium stable isotopes as a potential geochemical tool in agronomy–constraints and opportunities, Chemical Geology. https://doi.org/10.1016/.j.chemgeo.2022.121114

Uhlig, David; Berns, Anne E.; Wu, Bei; Amelung, Wulf (2023): Mean nutrient uptake depths of cereal crops change with compost incorporation into subsoil – evidence from 87Sr/86Sr ratios. Plant and Soil. https://doi.org/10.1007/s11104-023-06047-x

Table of contents

3. Data Description

The data herein were used to evaluate the success of subsoil management practices conducted from 2018 to 2020 at the central field sites (CF1 and CF2) of "Campus Klein Altendorf" (Rheinsberg, Germany). Subsoil management practices include deep loosening with and without the incorporation of biowaste compost and green waste compost, as well as using lucerne as deep rooting pre-crop. Subsoil managements are complemented by a control.

Presented are element concentrations of macronutrients (Ca, K, Mg, P), micronutrients (B, Cu, Fe, Mn, Zn), plant beneficial elements (Al, Co, Na, Ni, Si) and elements of non-nutritional character (Ba, Cd, Cr, Ga, Li, Pb, Rb, Sr, Ti) along with soil pH data, magnesium isotope compositions (δ^{26}Mg), and radiogenic strontium isotope ratios ($^{87}Sr/^{86}Sr$) of samples covering the soil-plant system of the agrosphere. Soil compartments include depth profiles of Luvisol of the easily exchangeable fraction of the soil (1M NH_4OAc extraction), and bulk soil ($Li_2B_4O_7$ fusion digests and microwave assisted sample digests). Plant compartments include bulk ear, bulk stem, and bulk leaf of winter wheat (*Triticum aestivum L.*) and spring barley (*Hordeum vulgare L.*) sampled at flowering and maturity stage. Chemical and isotope composition of bulk aboveground crop (shoot) are also presented. Finally, chemical and isotope compositions of compost and converter lime are provided.

Tables supplementary to the article, including data quality control, are provided in .pdf and .xlsx formats. In addition, data measured in the course of the study are also provided as machine readable ASCII files.

4. File description

Supplementary tables to Uhlig et al. (2022) are provided in .pdf and .xlsx formats. In addition, analytical data are provided as tab separated ASCII files. The first three rows in the ASCII files begin with "#" and contain licence and citation. In In all files, values that were not measured are marked with "n.d." and concentrations below limit of quantification are marked with "<LOQ".

4.1.File inventory

- **Table S1a** Chemical composition of pooled soil samples at central field trials ($Li_2B_4O_7$ fusion).
- **Table S1b** Loss on ignition corrected chemical composition of pooled soil samples at central field trials ($Li_2B_4O_7$ fusion).
- **Table S2a** Chemical composition of pooled soil samples at central field trials (microwave digestion).
- **Table S2b** Loss on ignition corrected chemical composition and magnesium and strontium isotope composition of pooled soil samples at central field trials (microwave digestion).
- **Table S3** Soil pH of pooled soil samples at central field trials.
- **Table S4** Chemical and magnesium and strontium isotope composition of the exchangeable fraction (1M NH_4OAc) of pooled soil samples at central field trials.
- **Table S5** Chemical and magnesium and strontium isotope composition of plant samples at central field trials.

4.2.Soil samples

4.2.1. 2022-003_Uhlig Table S1a Chemical composition of pooled soil samples at central field trials ($Li_2B_4O_7$ fusion)

Column header	unit	Description
sample ID	dimensionless	Sample identifier used in this study
field site	dimensionless	Name of central field trial
crop species	dimensionless	Description of crop type
growing stage	dimensionless	Description of growing stage
year	dimensionless	Year of sampling
treatment	dimensionless	[a] Subsoil management practice
soil horizon	dimensionless	Type of soil horizon
mean depth	cm	Mean sampling depth
SiO2	wt%	[b] Oxide concentration of silicon
TiO2	wt%	[b] Oxide concentration of titanium
Al2O3	wt%	[b] Oxide concentration of aluminium
Fe2O3	wt%	[b] Oxide concentration of iron
MnO	wt%	[b] Oxide concentration of manganese
MgO	wt%	[b] Oxide concentration of magnesium
CaO	wt%	[b] Oxide concentration of calcium
Na2O	wt%	[b] Oxide concentration of sodium
K2O	wt%	[b] Oxide concentration of potassium
P2O5	wt%	[b] Oxide concentration of phosphorus
LOI	wt%	Loss on ignition
Sum	wt%	Sum of oxide concentrations and LOI
Ba	ppm	[c] Barium concentration
Cd	ppm	[c] Cadmium concentration
Co	ppm	[c] Cobalt concentration
Cr	ppm	[c] Cadmium concentration
Pb	ppm	[c] Lead concentration
Sr	ppm	[c] Strontium concentration
Zn	ppm	[c] Zinc concentration

[a] C=control, DL=deep loosening, DLB=deep loosening with incorporation of biowaste compost, DLG=deep loosening with incorporation of green waste compost, C luc.=control with lucerne as pre-crop, DLB luc.=deep loosening with incorporation of biowaste compost and lucerne as pre-crop.

[b] Raw data (major elements, measured with ICP-OES).

[c] Raw data (trace elements, measured with ICP-OES).

4.2.2. 2022-003_Uhlig Table S1b Loss on ignition corrected chemical composition of pooled soil samples at central field trials ($Li_2B_4O_7$ fusion)

Column header	unit	Description
sample ID	dimensionless	Sample identifier used in this study
field site	dimensionless	Name of central field trial
crop species	dimensionless	Description of crop type
growing stage	dimensionless	Description of growing stage
year	dimensionless	Year of sampling
treatment	dimensionless	[a] Subsoil management practice
soil horizon	dimensionless	Type of soil horizon
mean depth	cm	Mean sampling depth
SiO2	wt%	[b] Oxide concentration of silicon
TiO2	wt%	[b] Oxide concentration of titanium
Al2O3	wt%	[b] Oxide concentration of aluminium
Fe2O3	wt%	[b] Oxide concentration of iron
MnO	wt%	[b] Oxide concentration of manganese
MgO	wt%	[b] Oxide concentration of magnesium
CaO	wt%	[b] Oxide concentration of calcium
Na2O	wt%	[b] Oxide concentration of sodium
K2O	wt%	[b] Oxide concentration of potassium
P2O5	wt%	[b] Oxide concentration of phosphorus
Sum	wt%	Sum of oxide concentrations and LOI
Ba	ppm	[c] Barium concentration
Cd	ppm	[c] Cadmium concentration
Co	ppm	[c] Cobalt concentration
Cr	ppm	[c] Chromium concentration
Pb	ppm	[c] Lead concentration
Sr	ppm	[c] Strontium concentration
Zn	ppm	[c] Zinc concentration

[a] C=control, DL=deep loosening, DLB=deep loosening with incorporation of biowaste compost, DLG=deep loosening with incorporation of green waste compost, C luc.=control with lucerne as pre-crop, DLB luc.=deep loosening with incorporation of biowaste compost and lucerne as pre-crop.

[b] LOI corrected data (major elements, measured with ICP-OES).

[c] LOI corrected data (trace elements, measured with ICP-OES).

4.2.3. 2022-003_Uhlig Table S2a Chemical composition of pooled soil samples at central field trials (microwave digestion)

Column header	unit	Description
sample ID	dimensionless	Sample identifier used in this study
field site	dimensionless	Name of central field trial
crop species	dimensionless	Description of crop type
growing stage	dimensionless	Description of growing stage
year	dimensionless	Year of sampling
treatment	dimensionless	[a] Subsoil management practice
soil horizon	dimensionless	Type of soil horizon
mean depth	cm	Mean sampling depth
SiO2	wt%	[b] Oxide concentration of silicon
TiO2	wt%	[b] Oxide concentration of titanium
Al2O3	wt%	[b] Oxide concentration of aluminium
Fe2O3	wt%	[b] Oxide concentration of iron
MnO	wt%	[b] Oxide concentration of manganese
MgO	wt%	[b] Oxide concentration of magnesium
CaO	wt%	[b] Oxide concentration of calcium
Na2O	wt%	[b] Oxide concentration of sodium
K2O	wt%	[b] Oxide concentration of potassium
P2O5	wt%	[b] Oxide concentration of phosphorus
LOI	wt%	Loss on ignition
B	ppm	[c] Boron concentration
Ba	ppm	[c] Barium concentration
Co	ppm	[c] Cobalt concentration
Cr	ppm	[c] Chromium concentration
Cu	ppm	[c] Copper concentration
Ga	ppm	[c] Gallium concentration
Li	ppm	[c] Lithium concentration
Ni	ppm	[c] Nickel concentration
Rb	ppm	[c] Rubidium concentration
Sr	ppm	[c] Strontium concentration
Zn	ppm	[c] Zinc concentration

[a] C=control, DL=deep loosening, DLB=deep loosening with incorporation of biowaste compost, DLG=deep loosening with incorporation of green waste compost, C luc.=control with lucerne as pre-crop, DLB luc.=deep loosening with incorporation of biowaste compost and lucerne as pre-crop.

[b] Raw data (major oxides, measured with ICP-MS).

[c] Raw data (trace elements, measured with ICP-MS).

4.2.4. 2022-003_Uhlig Table S2b Loss on ignition corrected chemical composition and magnesium and strontium isotope composition of pooled soil samples at central field trials (microwave digestion)

Column header	unit	Description
sample ID	dimensionless	Sample identifier used in this study
field site	dimensionless	Name of central field trial
crop species	dimensionless	Description of crop type
growing stage	dimensionless	Description of growing stage
year	dimensionless	Year of sampling
treatment	dimensionless	[a] Subsoil management practice
soil horizon	dimensionless	Type of soil horizon
mean depth	cm	Mean sampling depth
SiO2	wt%	[b] Oxide concentration of silicon
TiO2	wt%	[b] Oxide concentration of titanium
Al2O3	wt%	[b] Oxide concentration of aluminium
Fe2O3	wt%	[b] Oxide concentration of iron
MnO	wt%	[b] Oxide concentration of manganese
MgO	wt%	[b] Oxide concentration of magnesium
CaO	wt%	[b] Oxide concentration of calcium
Na2O	wt%	[b] Oxide concentration of sodium
K2O	wt%	[b] Oxide concentration of potassium
P2O5	wt%	[b] Oxide concentration of phosphorus
B	ppm	[c] Boron concentration
Ba	ppm	[c] Barium concentration
Co	ppm	[c] Cobalt concentration
Cr	ppm	[c] Chromium concentration
Cu	ppm	[c] Copper concentration
Ga	ppm	[c] Gallium concentration
Li	ppm	[c] Lithium concentration
Ni	ppm	[c] Nickel concentration
Rb	ppm	[c] Rubidium concentration
Sr	ppm	[c] Strontium concentration
Zn	ppm	[c] Zinc concentration
δ26Mg	‰	[d] Magnesium isotope ratio of ^{26}Mg to ^{24}Mg expressed in common delta notation
2SD	‰	[d] Uncertainty of δ^{26}Mg
δ25Mg	‰	[d] Magnesium isotope ratio of ^{25}Mg to ^{24}Mg expressed in common delta notation
2SD	‰	[d] Uncertainty of δ^{25}Mg
Δ25Mg	‰	[d] Deviation of δ^{25}Mg from the equilibrium isotope fractionation line in the three-isotope space calculated following (Young and Galy (2004)
n	dimensionless	[d] Number of Mg isotope mass spectrometry analyses
87Sr/86Sr	dimensionless	[d] Strontium isotope ratio of radiogenic ^{87}Sr to stable ^{86}Sr
2SE	dimensionless	[d] Uncertainty of ^{87}Sr/^{86}Sr

[a] C=control, DL=deep loosening, DLB=deep loosening with incorporation of biowaste compost, DLG=deep loosening with incorporation of green waste compost, C luc.=control with lucerne as pre-crop, DLB luc.=deep loosening with incorporation of biowaste compost and lucerne as pre-crop.

[b] LOI corrected data (major oxides, measured with ICP-MS).

[c] LOI corrected data (trace elements, measured with ICP-MS).

[d] MC-ICP-MS analyses.

4.2.5. 2022-003_Uhlig Table S3 Soil pH of pooled soil samples at central field trials

Column header	unit	Description
sample ID	dimensionless	Sample identifier used in this study
field site	dimensionless	Name of central field trial
crop species	dimensionless	Description of crop type
growing stage	dimensionless	Description of growing stage
year	dimensionless	Year of sampling
treatment	dimensionless	[a] Subsoil management practice
soil horizon	dimensionless	Type of soil horizon
mean depth	cm	Mean sampling depth
soil pH (CaCl2)	dimensionless	Soil pH measured in a suspension of 0.01M $CaCl_2$ and soil

[a] C=control, DL=deep loosening, DLB=deep loosening with incorporation of biowaste compost, DLG=deep loosening with incorporation of green waste compost, C luc.=control with lucerne as pre-crop, DLB luc.=deep loosening with incorporation of biowaste compost and lucerne as pre-crop.

4.2.6. 2022-003_Uhlig Table S4 Chemical and magnesium and strontium isotope composition of the exchangeable fraction (1M NH_4OAc) of pooled soil samples at central field trials

Column header	unit	Description
sample ID	dimensionless	Sample identifier used in this study
field site	dimensionless	Name of central field trial
crop species	dimensionless	Description of crop type
growing stage	dimensionless	Description of growing stage
year	dimensionless	Year of sampling
treatment	dimensionless	[a] Subsoil management practice
soil horizon	dimensionless	Type of soil horizon
mean depth	cm	Mean sampling depth
Ba	ppm	[b] Barium concentration
Ca	ppm	[b] Calcium concentration
Fe	ppm	[b] Iron concentration
K	ppm	[b] Potassium concentration
Li	ppb	[b] Lithium concentration
Mg	ppm	[b] Magnesium concentration
Mn	ppm	[b] Manganese concentration
Na	ppm	[b] Sodium concentration
P	ppm	[b] Phosphorus concentration
Rb	ppm	[b] Rubidium concentration

Column header	unit	Description
Sr	ppm	[b] Strontium concentration
Zn	ppm	[b] Zinc concentration
δ26Mg	‰	[c] Magnesium isotope ratio of ^{26}Mg to ^{24}Mg expressed in common delta notation
2SD	‰	[c] Uncertainty of $\delta^{26}Mg$
δ25Mg	‰	[c] Magnesium isotope ratio of ^{25}Mg to ^{24}Mg expressed in common delta notation
2SD	‰	[c] Uncertainty of $\delta^{25}Mg$
Δ25Mg	‰	[c] Deviation of $\delta^{25}Mg$ from the equilibrium isotope fractionation line in the three-isotope space calculated following (Young and Galy (2004)
n	dimensionless	[c] Number of Mg isotope mass spectrometry analyses
87Sr/86Sr	dimensionless	[c] Strontium isotope ratio of radiogenic ^{87}Sr to stable ^{86}Sr
2SE	dimensionless	[c] Uncertainty of $^{87}Sr/^{86}Sr$

[a] C=control, DL=deep loosening, DLB=deep loosening with incorporation of biowaste compost, DLG=deep loosening with incorporation of green waste compost, C luc.=control with lucerne as pre-crop, DLB luc.=deep loosening with incorporation of biowaste compost and lucerne as pre-crop.

[b] ICP-MS analyses.

[c] MC-ICP-MS analyses.

4.3. Plant samples

4.3.1. 2022-003_Uhlig Table S5 Chemical and magnesium and strontium isotope composition of plant samples at central field trials

Column header	unit	Description
sample ID	dimensionless	Sample identifier used in this study
field site	dimensionless	Name of central field trial
crop species	dimensionless	Description of crop type
growing stage	dimensionless	Description of growing stage
year	dimensionless	Year of sampling
plant organ	dimensionless	Description of plant organ
field repetition - treatment	dimensionless	[a] Field replicate and subsoil management practice
biomass	g	Total mass of plant organ
K	ppm	[b] Potassium concentration
Ca	ppm	[b] Calcium concentration

Column header	unit	Description
Mg	ppm	[b] Magnesium concentration
P	ppm	[b] Phosphorus concentration
Fe	ppm	[c] Iron concentration
Mn	ppm	[c] Manganese concentration
Zn	ppm	[c] Zinc concentration
Cu	ppm	[c] Copper concentration
B	ppm	[c] Boron concentration
Na	ppm	[d] Sodium concentration
Al	ppm	[d] Aluminium concentration
Co	ppm	[d] Cobalt concentration
Ba	ppm	[e] Barium concentration
Sr	ppm	[e] Strontium concentration
Ti	ppm	[e] Titanium concentration
Cr	ppb	[e] Chromium concentration
Li	ppb	[e] Lithium concentration
δ26Mg	‰	[f] Magnesium isotope ratio of ^{26}Mg to ^{24}Mg expressed in common delta notation
2SD	‰	[f] Uncertainty of δ^{26}Mg
δ25Mg	‰	[f] Magnesium isotope ratio of ^{25}Mg to ^{24}Mg expressed in common delta notation
2SD	‰	[f] Uncertainty of δ^{25}Mg
Δ25Mg	‰	[f] Deviation of δ^{25}Mg from the equilibrium isotope fractionation line in the three-isotope space calculated following (Young and Galy (2004)
n	dimensionless	[f] Number of Mg isotope mass spectrometry analyses
87Sr/86Sr	dimensionless	[f] Strontium isotope ratio of radiogenic ^{87}Sr to stable ^{86}Sr
2SE	dimensionless	[f] Uncertainty of ^{87}Sr/^{86}Sr

[a] C=control, DL=deep loosening, DLB=deep loosening with incorporation of biowaste compost, DLG=deep loosening with incorporation of green waste compost, C luc.=control with lucerne as pre-crop, DLB luc.=deep loosening with incorporation of biowaste compost and lucerne as pre-crop.

[b] Macronutrients (measured with ICP-OES).

[c] Micronutrients (Fe, Mn, Zn measured with ICP-OES; Cu, B measured with ICP-MS).

[d] Beneficial elements (measured with ICP-OES).

[e] Non-nutritive elements (measured with ICP-MS).

[f] MC-ICP-MS analyses.

5. References

Uhlig, D., Wu, B., Berns, A.E., Amelung, W. (2022): Magnesium stable isotopes as a potential geochemical tool in agronomy–constraints and opportunities, Chemical Geology. https://doi.org/10.1016/.j.chemgeo.2022.121114

Uhlig, David; Berns, Anne E.; Wu, Bei; Amelung, Wulf (2023): Mean nutrient uptake depths of cereal crops change with compost incorporation into subsoil – evidence from 87Sr/86Sr ratios. Plant and Soil. https://doi.org/10.1007/s11104-023-06047-x

Young ED, Galy A (2004) The Isotope Geochemistry and Cosmochemistry of Magnesium. In: Reviews in Mineralogy and Geochemistry. pp 197–230