

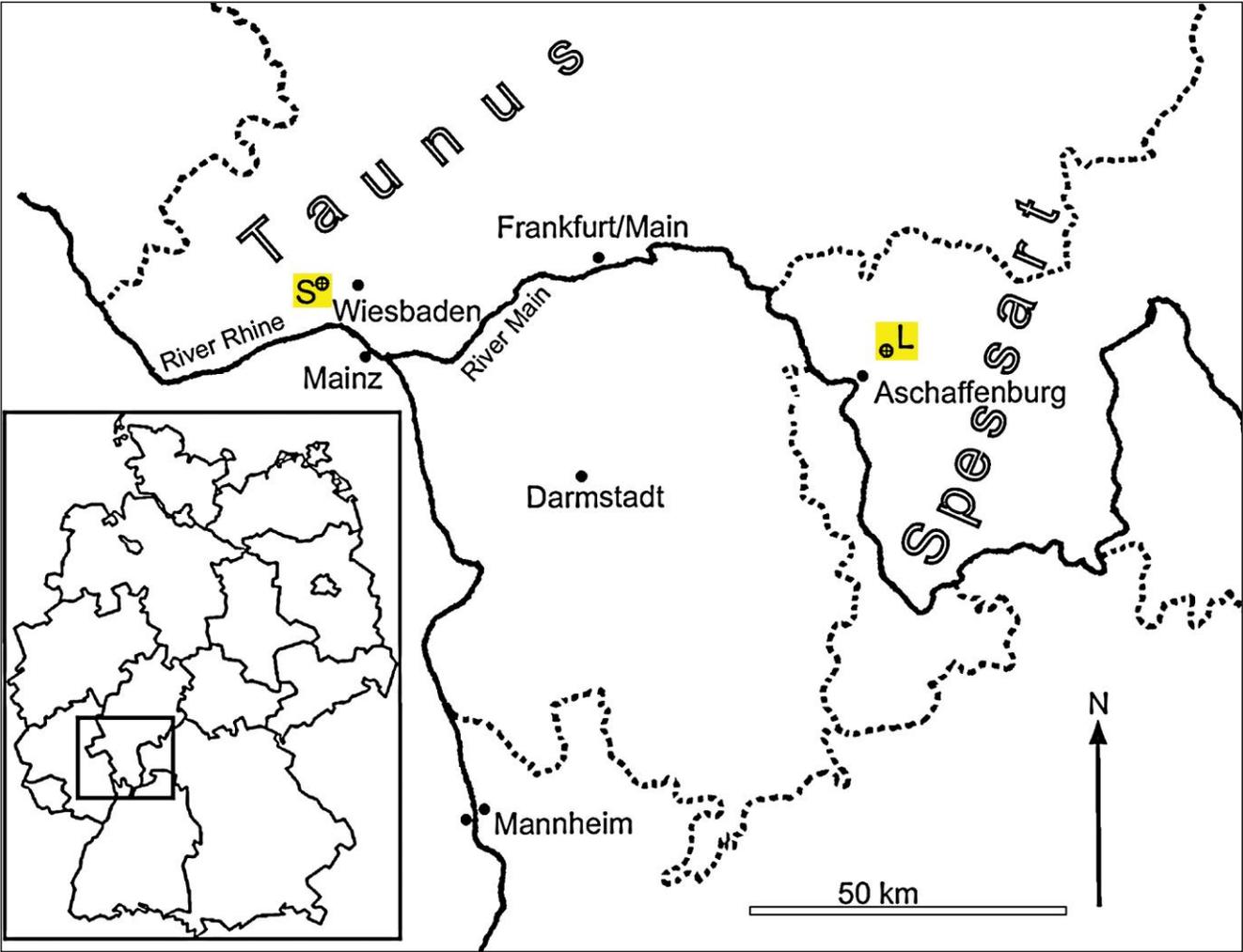
# **Speciation and Mobility of Arsenic in Agricultural Lime**

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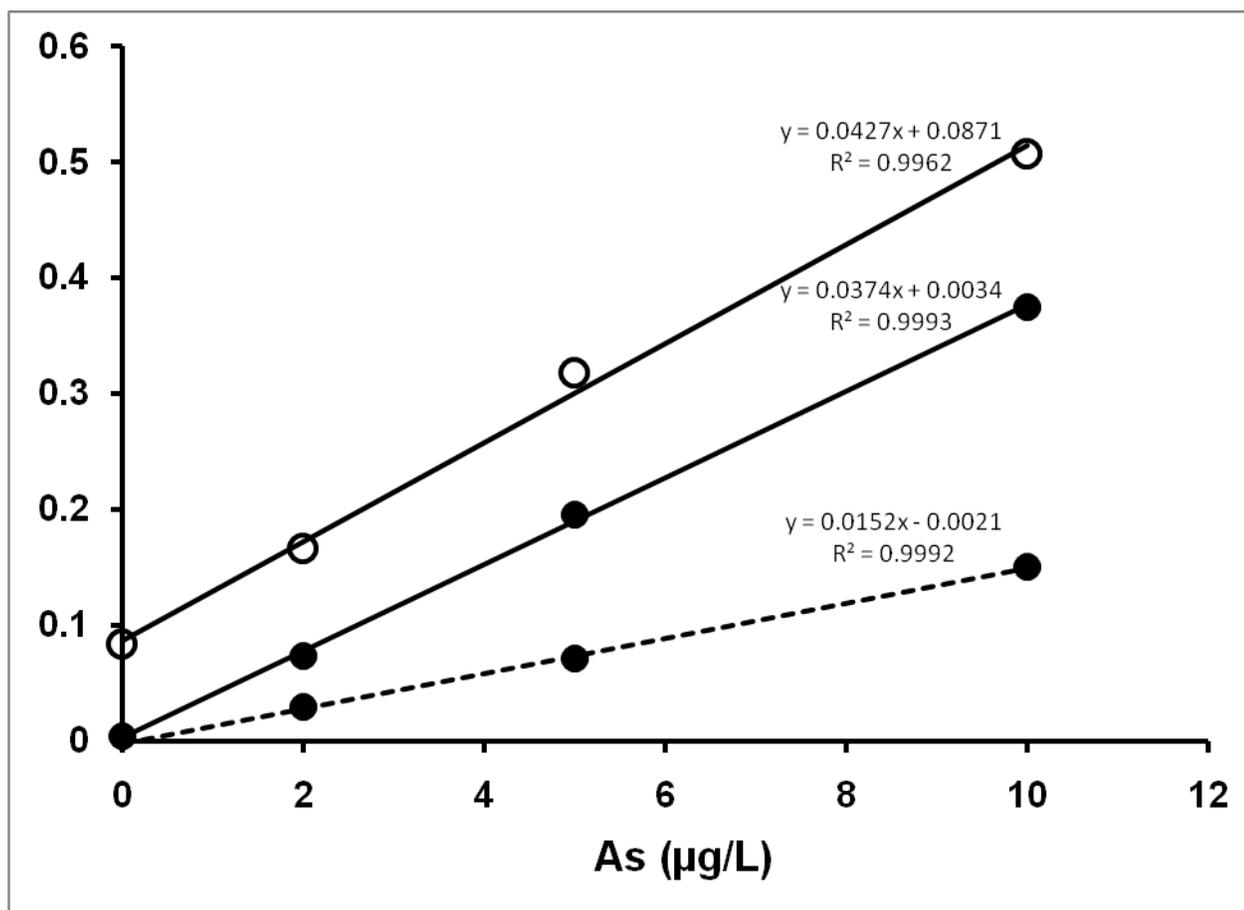
## **Supplemental Information**

Including 6 Figures and 1 Table on 5 pages

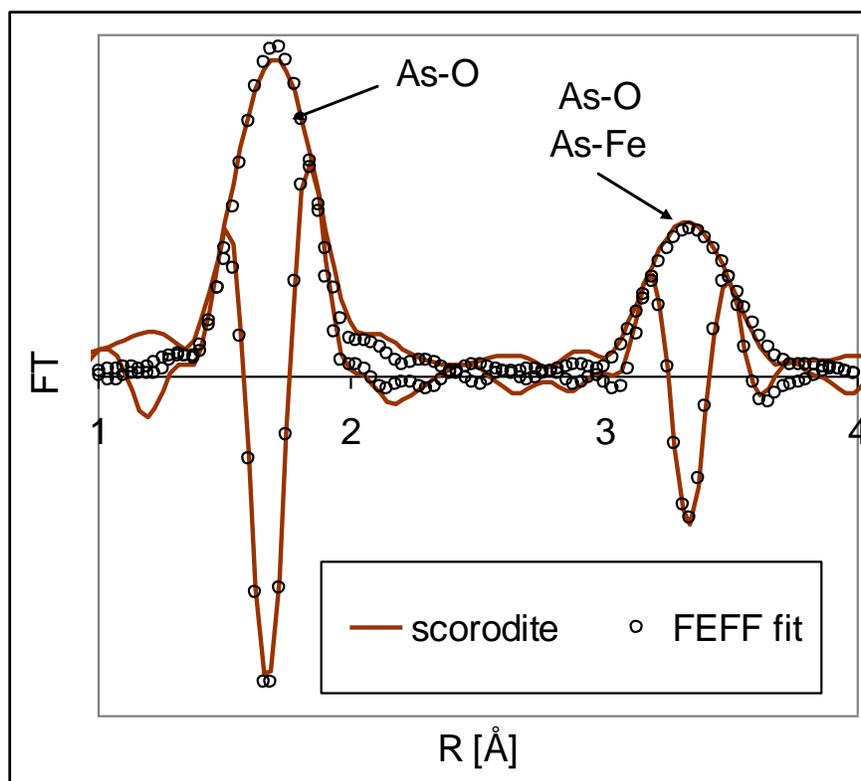
Supplemental Figure 1. Location of limestone (L) and soil (S) sampling sites within Germany (inlet map).



Supplemental Figure 2. Calibration plots demonstrating analytical problem with hydride generation atomic absorption spectroscopy (HG-AAS). Dissolved transition metals like Fe interfere in the HG-AAS determination of arsenic in geologic samples. Interferences by the enhanced Fe concentrations led to a double as high As concentration for the strongly reducing step 4, if no masking reagents such as cysteine were used in the HG-AAS measurements as suggested already by Näykki et al. (2001). The plot shows standard calibration curves (black dots) with (solid line) and without (dotted line) 1% cysteine masking reagent, together with the standard addition curve (open dots). The slope of the latter standard calibration curve differs to that of the standard addition curve for the same sample which is indicative for the interference effect.



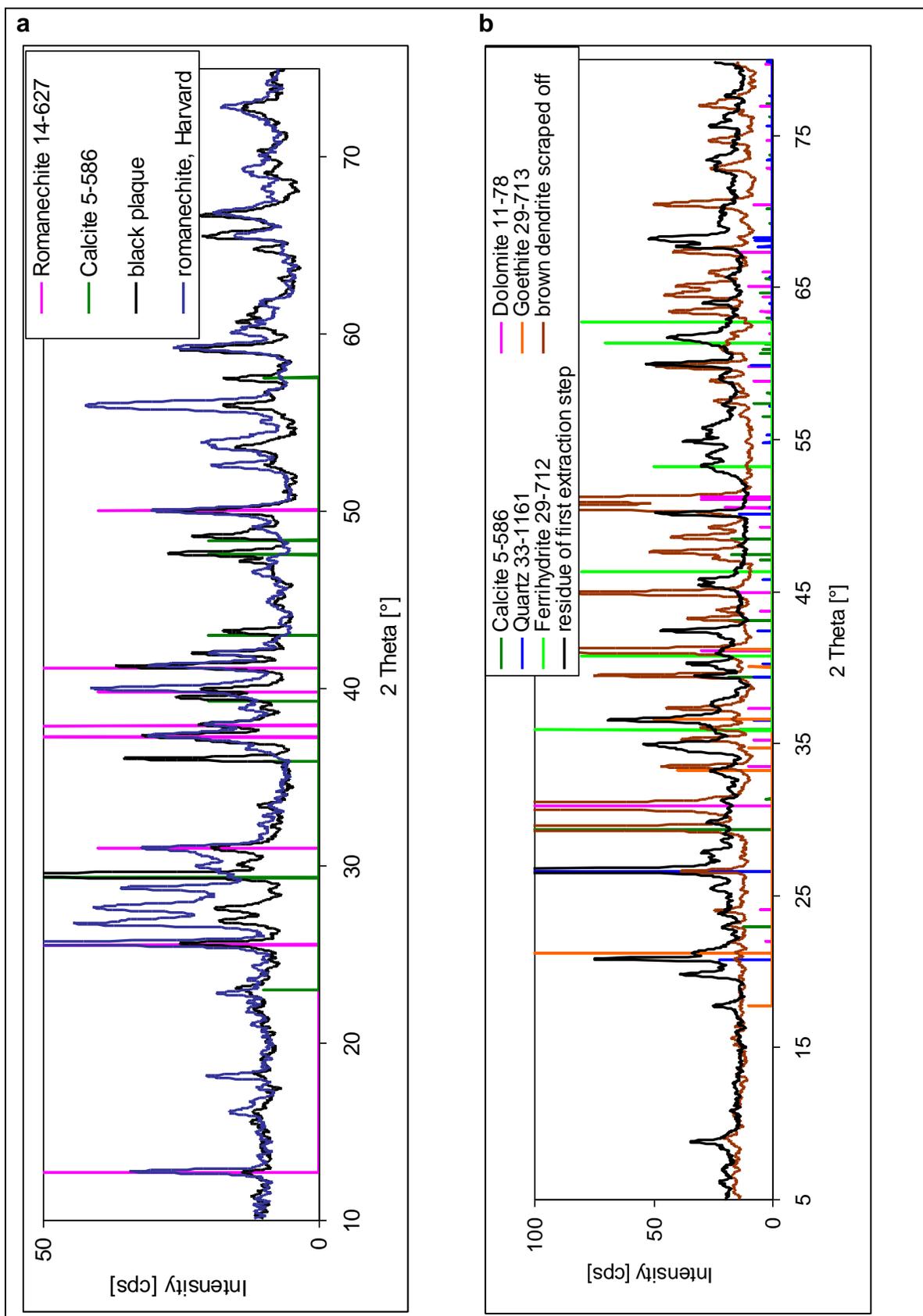
Supplemental Figure 3. RDF from bulk As EXAFS results of scorodite with FEFF fit (circles) of the scorodite crystal structure model.



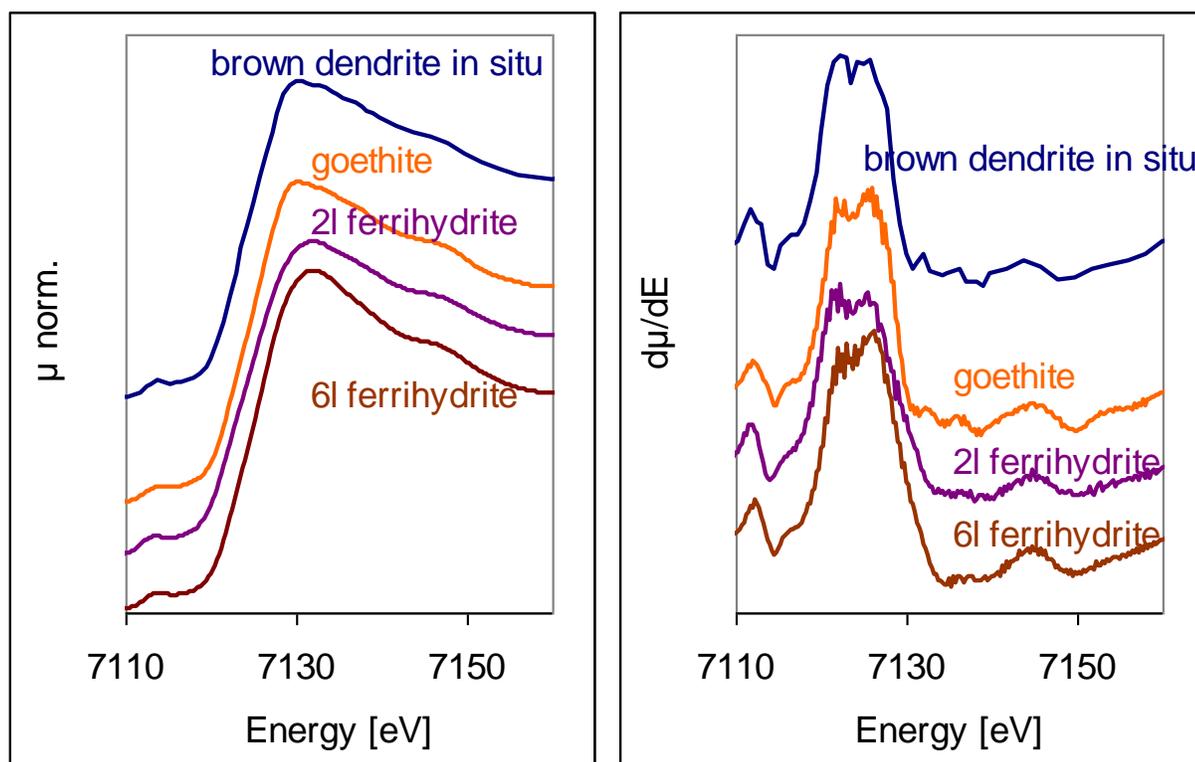
Supplemental Table 1. Parameters resulting from the FEFF fit of scorodite crystal structure data to the As bulk EXAFS spectra from scorodite ( $\Delta E_0 = 6.94 \pm 1.37$  eV; r-factor = 0.046). The highest correlations were found between the path lengths of As-O(2) and As-Fe (-0.88) and between the path length of As-O(1) and  $\Delta E_0$  (0.79).

Scattering path	$N$	$\sigma^2$ [ $\text{\AA}^2$ ]	$R$ [ $\text{\AA}$ ]
As-O(1)	4.0	$0.0020 \pm 0.0003$	$1.69 \pm 0.005$
As-O(2)	2.0	$0.0020 \pm 0.0003$	$3.34 \pm 0.098$
As-Fe	2.0	$0.0022 \pm 0.0021$	$3.37 \pm 0.022$

Supplemental Figure 4. Bulk powder diffraction patterns of (a) black plaque + reference and (b) brown dendrite, including reference patterns from the PDF2 database.



Supplemental Figure 5. Fe  $\mu$ -XANES results from measurements of Fe oxides in dendrites (spots 1 and 2) and of known reference samples.



Supplemental Figure 6. As K-edge  $\mu$ -XANES results from measurements of Fe- and As-rich spots in dendrites.

