

Supplemental Information to *Characterization of Iron Speciation in Single Particles using XANES Spectroscopy and Micro X-ray Fluorescence Measurements: Investigating the Relationship between Iron Speciation and Fractional Iron Solubility*

II. Tables

- i. Table S1** Fe mineral standards
- ii. Table S2** Total Fe concentration measured in Southeastern US during 2008

III. Figures

- i. Figure S1** Example of features in XANES spectra
- ii. Figure S2** Histogram of pre-edge centroid positions

Supplemental Information: Tables

Table S1. Fe Mineral Standards

<i>Sample</i>	<i>Mineral Type</i>	<i>Origin</i>
Augite	Iron-aluminosilicate	Mineralogical Research Co. Gjerstad, Norway
Biotite	Iron-aluminosilicate	Mineralogical Research Co. Bancroft, Ontario
Iron (II) Oxalate	Iron Organic	Sigma-Aldrich, Product 307726
Pyrite	Iron Sulfide	Mineralogical Research Co. Huanzala, Dept. of Huanco, Peru
Iron (II) Sulfate	Sulfur-containing Iron	Sigma-Aldrich, Product 215422
Iron (III) Sulfate	Sulfur-containing Iron	Sigma-Aldrich, Product 307718
Goethite	Iron Oxide	Cartersville, Georgia USA
Hematite	Iron Oxide	Mineralogical Research Co. Butte, Montana USA

Table S2. Total Fe concentration measured in Southeastern US during 2008

<i>Site</i>	<i>Season</i>	<i>Mean</i>	<i>Median</i>	<i>Max</i>	<i>Min</i>	<i>Stdev</i>	<i>N</i>
Urban ^a	Summer	98.6	81.3	1030.0	15.4	66.2	154
	Winter	56.8	46.9	395.0	0.0	37.7	194
Atlanta, GA South Dekalb ^b	Summer	111.2	95.8	248.0	24.6	51.6	25
	Winter	61.2	45.8	172.0	6.5	46.8	25
Atlanta, GA Jefferson St. ^c	Summer	61.2	45.8	172.0	6.5	46.8	22
	Winter	49.0	36.0	184.8	2.7	34.6	73
Rural ^d	Summer	75.0	39.2	407.8	12.9	10.1	69
	Winter	22.2	20.5	74.9	2.7	20.0	71
Yorkville, GA ^{c,e}	Summer	54.1	33.8	331.2	10.5	66.3	29
	Winter	22.1	20.4	61.5	2.7	11.7	28

*Concentrations measured in ng/m³

- a) Mean total Fe measurements from seven urban sites supported by the EPA Air Explorer Network, <http://www.epa.gov/airexplorer/index.html>
- b) Measurements supported by EPA Air Explorer Network, <http://www.epa.gov/airexplorer/index.html>
- c) Measurements supported by SEARCH study, <http://www.atmospheric-research.com/public/index.html>
- d) Mean total Fe measurements from four rural sites supported by the EPA Air Explorer Network, <http://www.epa.gov/airexplorer/index.html>
- e) Rural site northwest of Atlanta, GA

Supplemental Information: Figures

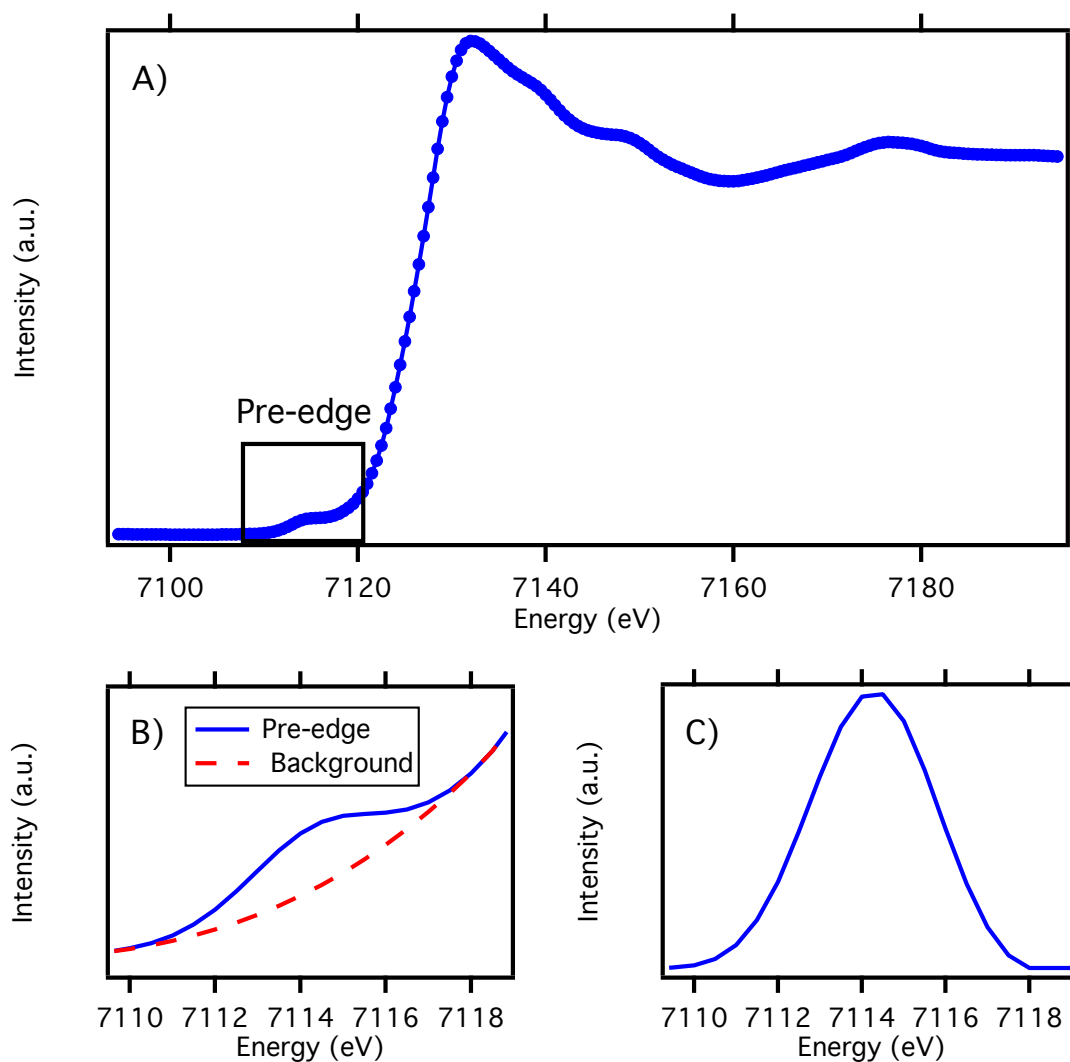


Figure S1. A) Example of XANES spectra. The black box represents the pre-edge feature used to determine iron oxidation state. B) Example of the pre-edge feature of XANES spectra (blue line) and interpolated cubic spline background (red dashed line) and C) Example of fitted pre-edge feature. Pre-edge centroid position is located at the maximum of the peak.

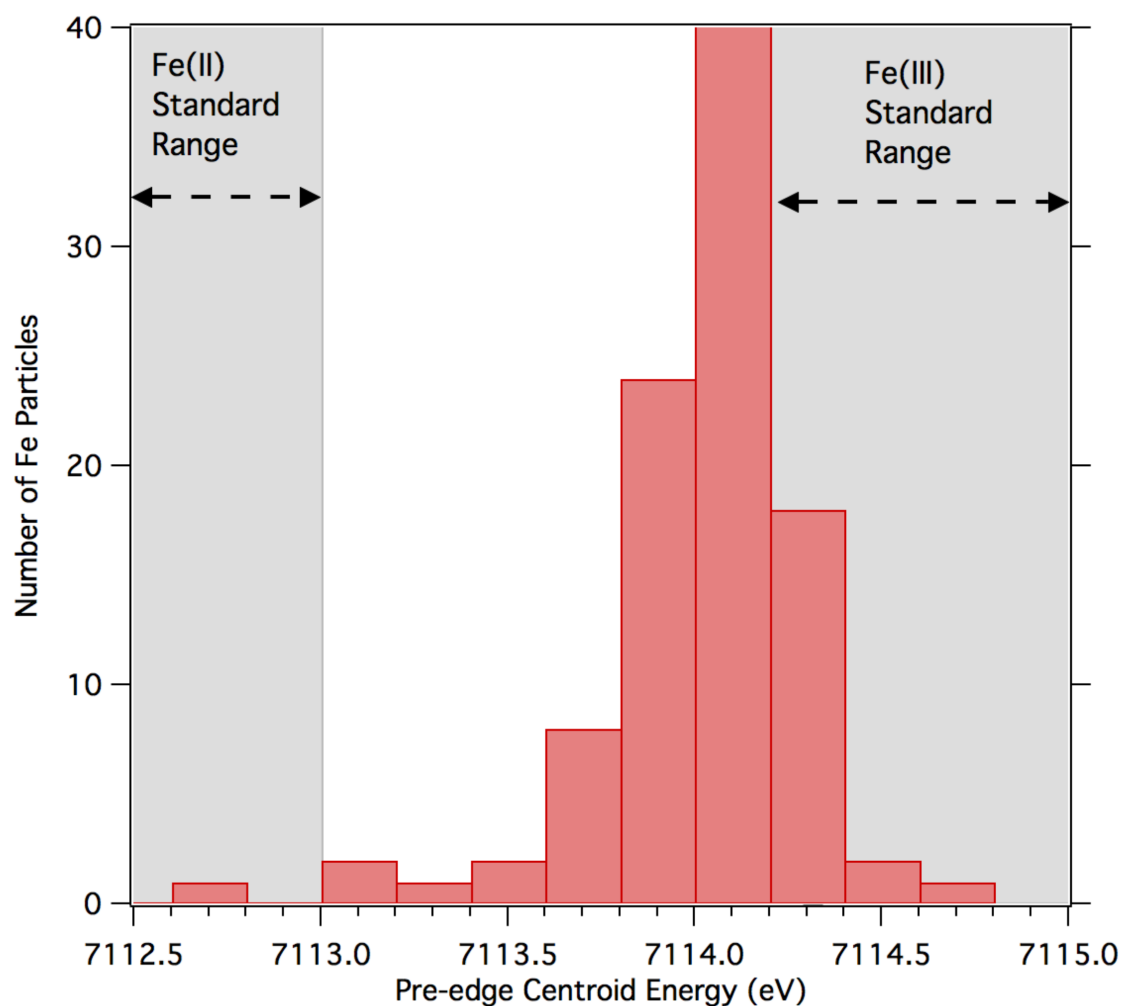


Figure S2. Histogram of pre-edge centroid energy positions determined from XANES spectra of individual iron particles from urban and rural sites is plotted. The gray shaded areas on the map represent the range of pre-edge centroid positions for common Fe(II) and Fe(III) minerals.