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Supplementary material

Vanadate complexation to ferrihydrite: X-ray absorption spectroscopy and CD-MUSIC modelling

Maja A. Larsson,[A] *Ingmar Persson,*[B] *Carin Sjöstedt*[A] *and Jon Petter Gustafsson*[A,C,D]

[A]Department of Soil and Environment, Swedish University of Agricultural Sciences, Box 7014, SE-750 07 Uppsala, Sweden.

[B]Department of Molecular Sciences, Swedish University of Agricultural Sciences, Box 7015, SE-750 07 Uppsala, Sweden.

[C]Division of Land and Water Resources Engineering, Royal Institute of Technology, Teknikringen 76, SE-100 44, Stockholm, Sweden.

[D]Corresponding author. Email: jon-petter.gustafsson@slu.se

A. Batch experiments

Table S1. Batch experiments performed with 2-line ferrihydrite and vanadate in a total of eight series[A]

Series[B]	*n* samples	Fe (mM)	V (μM)	P (μM)	Fe:V ratio	Fe:P ratio	pH range
L-1	11	0.3	50	-	6	-	3.21 – 9.53
R-1	14	0.3	50	-	6	-	3.06 – 9.87
L-2	13	1	50	-	20	-	4.65 – 9.88
R-2	17	1	50	-	20	-	3.02 – 10.10
L-3	14	3	50	-	60	-	5.31 – 10.30
R-3	15	3	50	-	60	-	4.15 – 10.21
L-4	16	3	5	-	600	-	3.09 – 10.49
L-5	16	1	50	200	20	5	3.10 – 10.47

[A]All samples had an ionic strength of 0.01 M added as $NaNO_3$. Either HNO_3 or NaOH was added to adjust the pH value.

[B]The R series were processed by M. Rasmus at KTH Royal Institute of Technology (KTH) in May 2009. The L series were prepared by M. A. Larsson at the Swedish University of Agricultural Sciences (SLU) in September 2009.

B. Results from vanadium K-edge XANES spectroscopy

Table S2. Pre-edge properties and K-edge positions of standards and ferrihydrite samples

Sample	Pre-edge peak			Main edge
	Area	Intensity	Centroid position (eV)	$E_{½}$(eV)[A]
Standards				
V_2O_5(s)	1.9	0.66	5469.4	5480.6
VO^{2+}(aq)	1.0	0.36	5469.9	5478.8
$H_2VO_4^-$(aq)	2.2	0.81	5469.8	5481.0
Ferrihydrite				
C	1.9	0.78	5469.9	5482.0
D	1.9	0.80	5469.6	5481.7
F	1.9	0.84	5469.7	5481.7

[A]$E_{½}$ = the energy on the main edge where the normalized intensity = 0.5.

C. Wavelet transform analysis

Calculation of Morlet wavelet transforms was made as described by Tiberg et al.[1]

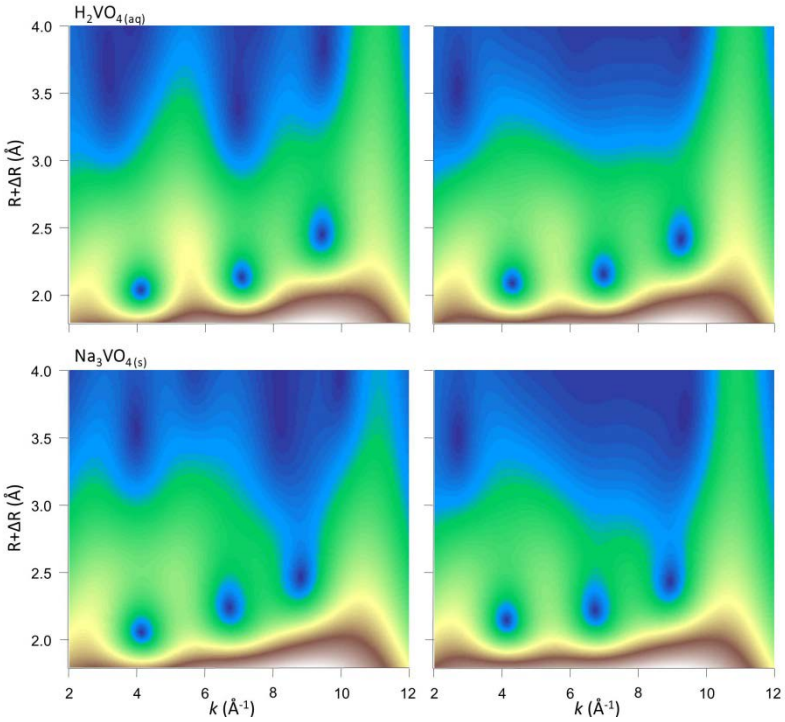

Fig. S1. Morlet wavelet transforms of k^3-weighted vanadium K-edge EXAFS spectra of vanadium laboratory standards, solid and dissolved vanadate samples (κ = 6, σ = 1). Experimental data (left) and modelled data (right).

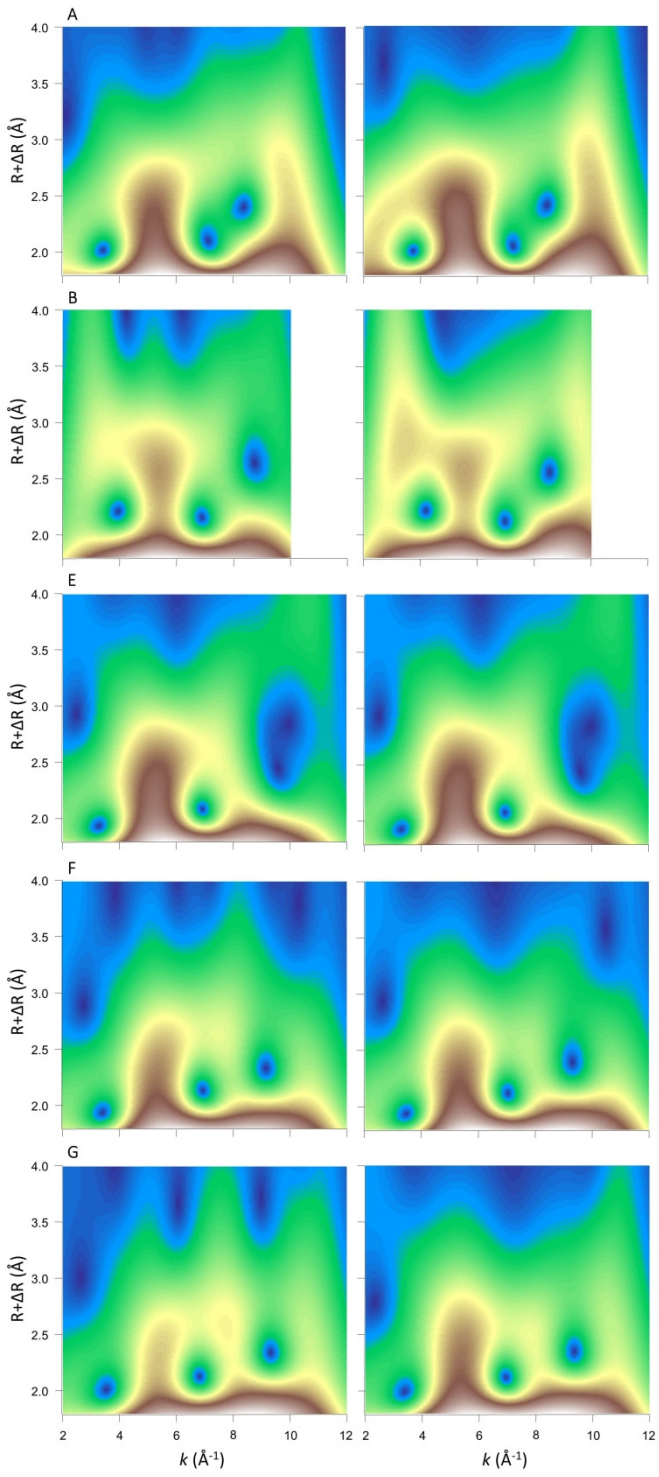

Fig. S2. Morlet wavelet transforms of k^3-weighted vanadium K-edge EXAFS spectra of samples A, B, E, F and G (κ = 6, σ = 1). Experimental data (left) and modelled data (right).

References

[1] C. Tiberg, C. Sjöstedt, I. Persson, J.P. Gustafsson, Phosphate effects on copper(II) and lead(II) sorption to ferrihydrite. *Geochim. Cosmochim. Acta* **2013,** *120*, 140.