Electronic Supplementary Material (ESI) for CrystEngComm.

Supplementary Materials

for

Incorporation of molybdenum(VI) in akaganéite (β-FeOOH) and the microbial reduction of Mo-akaganéite by *Shewanella loihica* PV-4

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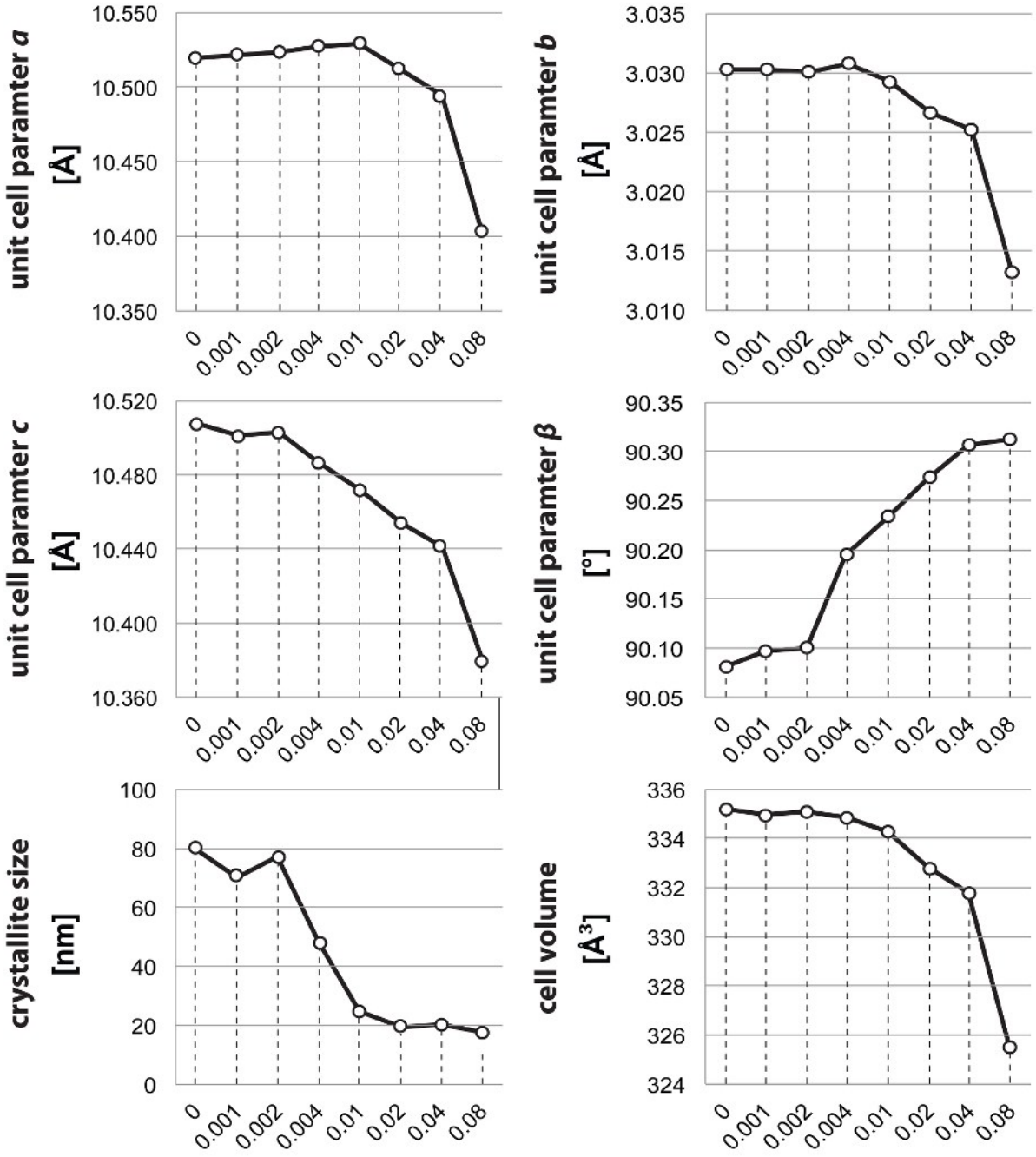

Figure 1S: Unit cell parameters, crystallite size and cell volume of Mo-free akaganéite (Mo_0) and Mo-akaganéite ($Mo_{0.001\text{-}Mo0.08}$) as determined by full profile fitting with the previously described akaganéite structure[1].

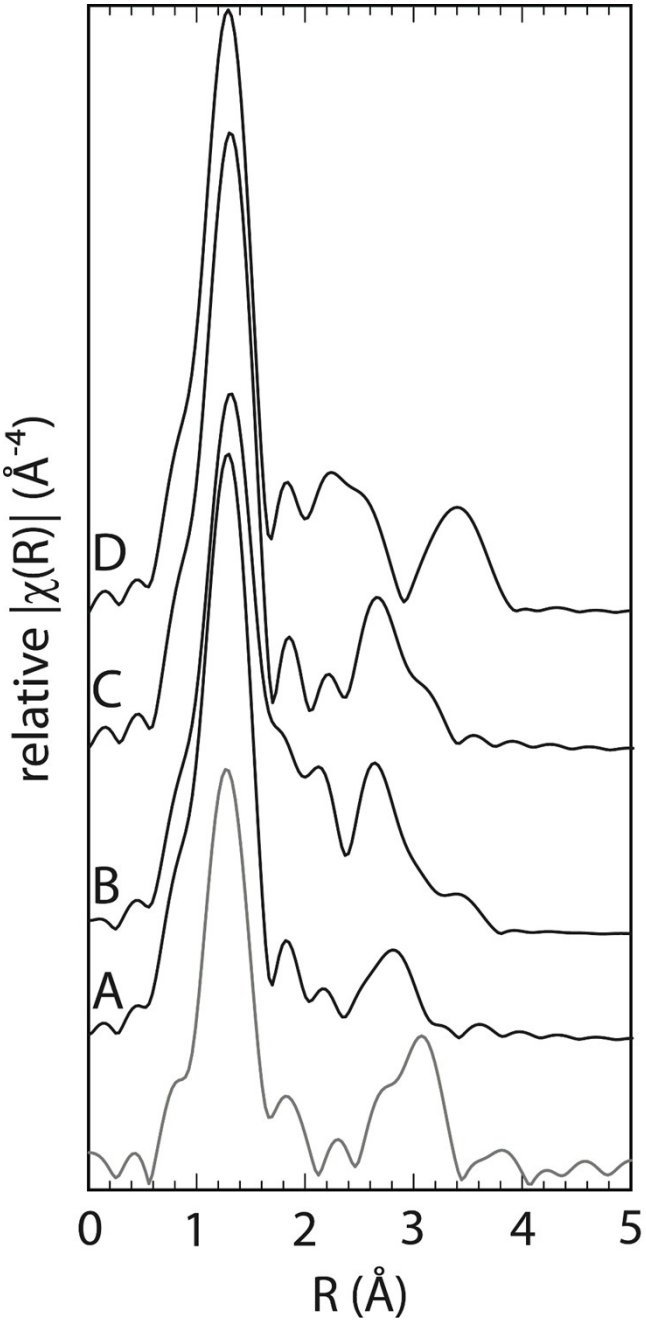

Figure 2S: Magnitude of the Fourier transform of Mo-bearing akaganéite at the Mo *K*-edge and simulation of Mo^{6+} tetrahedrally coordinated by oxygen at different positions in the akaganéite structure, including: A: bound to a single FeO_6-octahedron as monodentate complex to the akaganéite surface, B: bound to one FeO_6-octahedron as bidentate-mononuclear complex, C: bound to two FeO_6-octahedra as bidentate-binuclear complex and D: residing on the Cl^--position within the tunnel structure of akaganéite. For the simulation, all paths calculated by FEFF6[2] until 4 Å were included in the simulation. The coordination number remained unaltered, $\Delta E_0=0$, $\Delta r=0$, $\sigma_{\text{first shell}}=0.006$ and $\sigma_{\text{successive shells}}=0.008$.

REFERENCES

[1] J.E. Post, P.J. Heaney, R.B. Von Dreele, J.C. Hanson, *American Mineralogist,* 2003, ***88***, 782-788.

[2] M.J. de Leon, J.J. Rehr, S.I. Zabinsky, R.C. Albers, *Physical Review Letters,* 1991, ***B44***, 4146-4156.