Combined bioreduction and volatilization of SeVI by Stenotrophomonas bentonitica: Formation of trigonal selenium nanorods and methylated species

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SUPPLEMENTARY MATERIAL

Combined bioreduction and volatilization of Se^{VI} by the bacterium *Stenotrophomonas bentonitica*: formation of trigonal selenium nanorods and methylated species

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1. Materials and Methods

1.1. X-ray absorption spectroscopy (XAS) measurements

Experimentally, the ring was operated at 2.75 GeV in 8-bunch mode (100 mA). The optics consisted of a double-crystal monochromator with horizontal dynamical focusing set to the Si (220) crystals, and -coated mirrors for vertical focusing and rejection of higher harmonics set to the Si strips (Solari et al. 2009). Spectra were collected in fluorescence mode using a 13-element Ge detector (EG & G ORTEC, USA). Selenium references XAS data were collected in transmission mode. Data were processed following standard procedures by using EXAFSPAK. Background removal was performed by means of a pre-edge linear function. Atomic absorption was simulated with a square-spline function. The theoretical phase and amplitude functions used in data analysis were calculated with FEFF8 (Ankudinov and Ravel, 1998) using trigonal Se as atomic model. The amplitude reduction factor (S_0^2) was held constant at 1.0 for the FEFF8 calculation and extended x-ray absorption fine structure (EXAFS) fits. The shift in threshold energy, $\Delta E0$, was varied as a global parameter in the fits. The absorption threshold E0 was set to 12 658 eV using the peak of the first derivative near the absorption edge. Fitting was performed in R-space with a k-weight of 3. A k range of 4 to 13 $Å^{-1}$ was used for the $|\chi(R)|$ transform. The maximal systematic errors in the coordination number obtained by EXAFSPAK software could reach the value of 25% due to the strong correlation between the σ_2 value and the bond distance. However, the estimated deviations are calculated for the coordination number of each coordination sphere and could be much lower than the 25% as the case of those of the studied samples.

2. Supplementary Figures

Figure S1

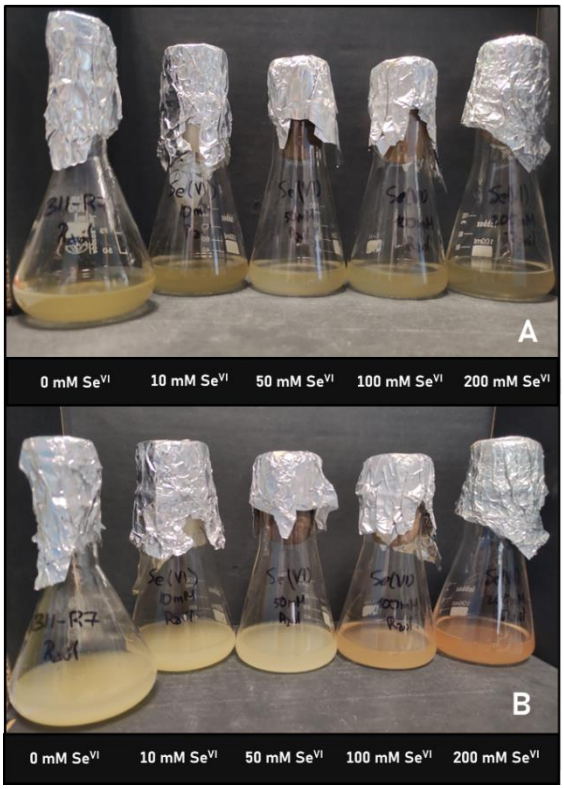

Figure S1. Cultures of *S. bentonitica* in LB broth supplemented with 0, 10, 50, 100, and 200 mM Se(VI) after 0 (A) and 48 hours (B).

Figure S2

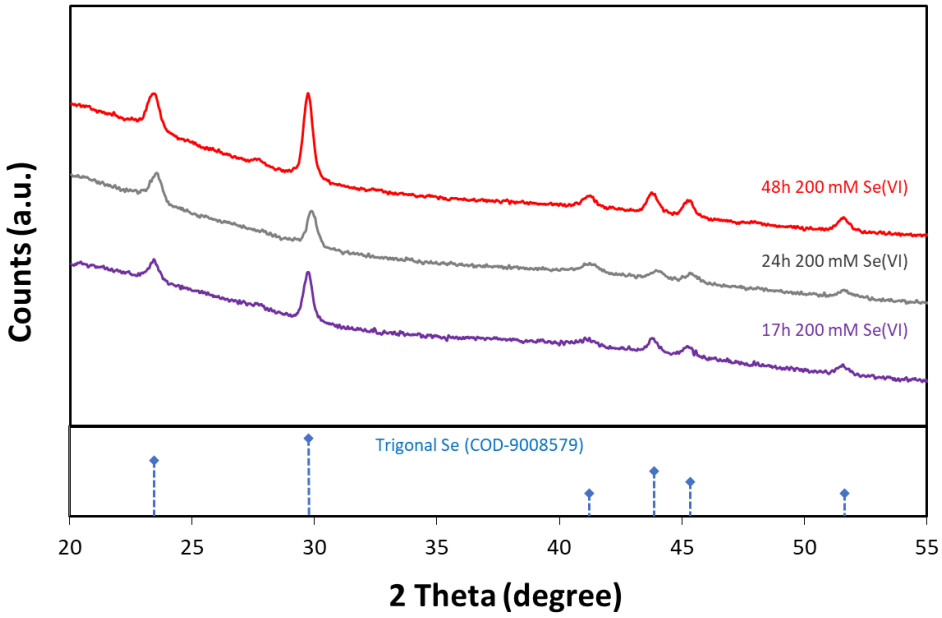

Figure S2. X-ray diffraction pattern of cultures of *S. bentonitica* supplemented with 200 mM Se(VI) after 17, 24, and 48h of incubation. Peaks for Se with a trigonal structure t-Se were detected as indicated the corresponding peaks for t-Se (COD-9008579) obtained from Crystallography Open Database (http://www.crystallography.net/cod/).

Figure S3

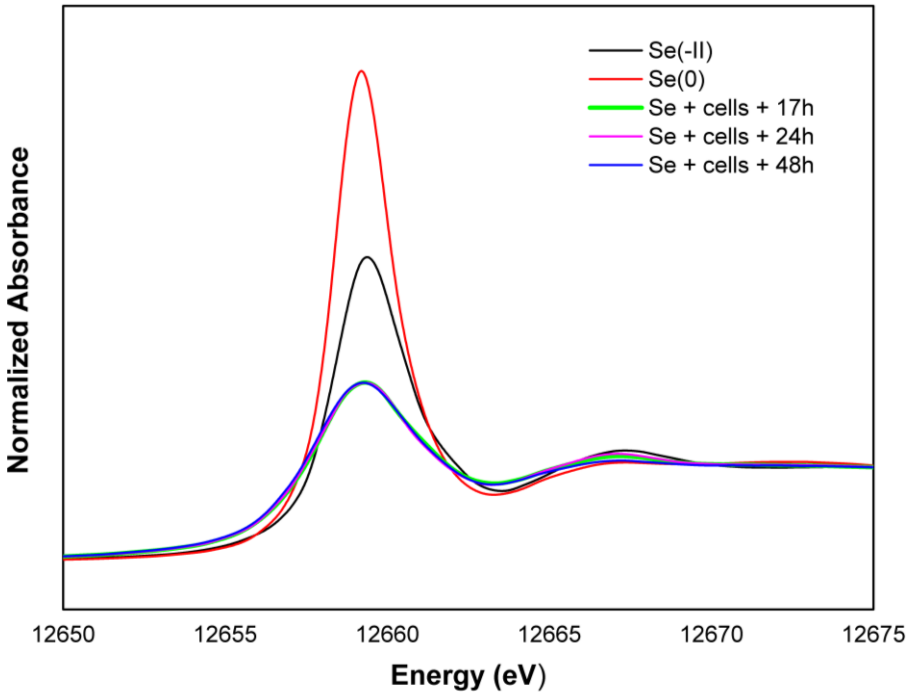

Figure S3. XANES spectra of Se(0) and Se(-II) references and the Se products samples after 17, 24, and 48h.

Figure S4

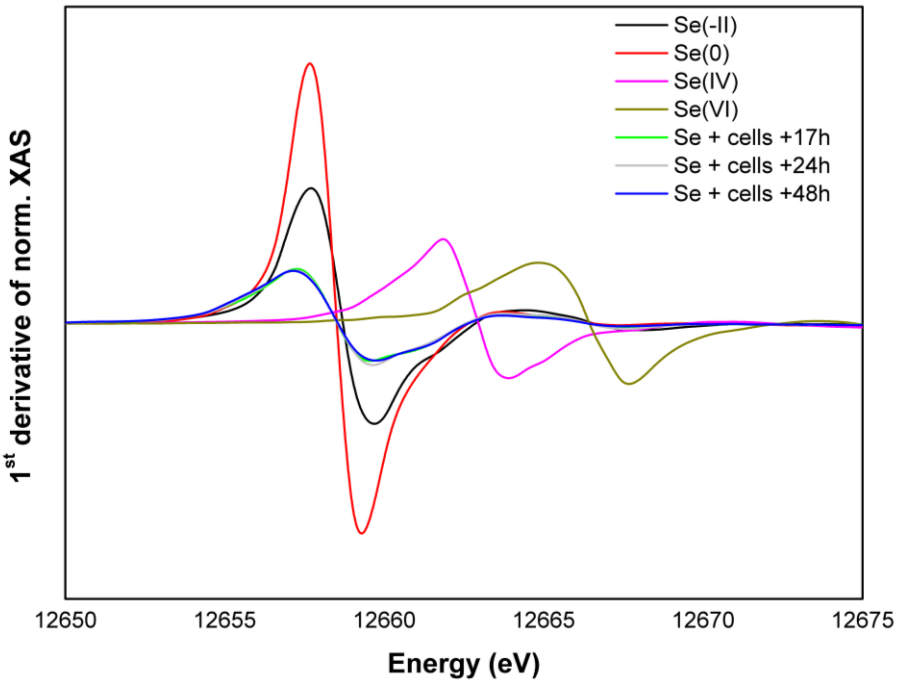

Figure S4. First derivative of the XANES spectra of Se reference compounds (A) and biogenic SeNPs samples produced by *S. bentonitica* at different incubation times (24, 72, and 144 h)

Figure S5

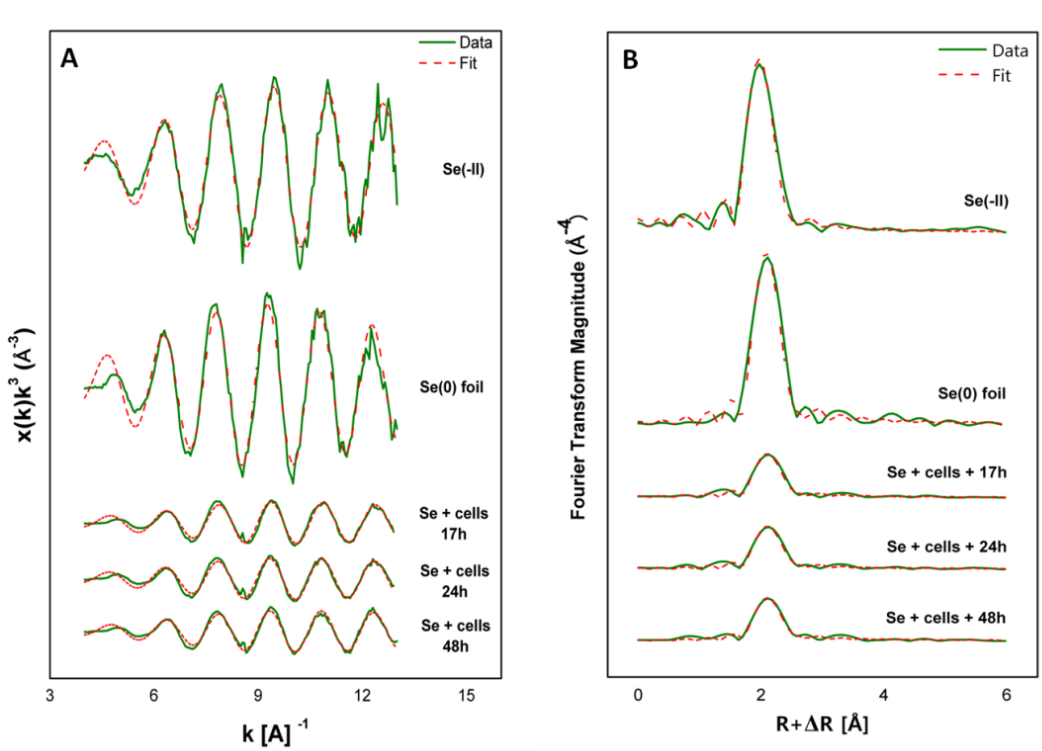

Figure S5. EXAFS (A) and their corresponding FT spectra (B) of Se reference compounds and *S. bentonitica* samples incubated with 200 mM Se(VI) at different incubation times (17, 24, and 48 h).

Figure S6

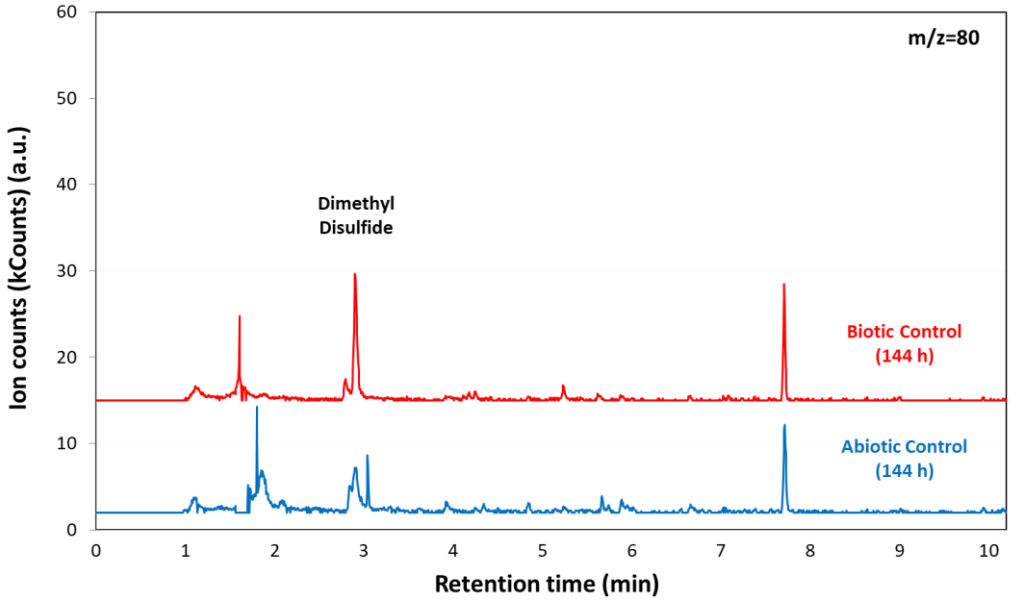

Figure S6. GC-MS chromatograms of the headspace gas non-treated cultures of *S. bentonitica* (biotic control) and Se(VI)-treated media (abiotic control) after 144 h of incubation. All GC-MS chromatograms were obtained by selecting the 80 m/z ion specific for selenium.

References

Ankudinov, A., & Ravel, B. (1998). Real-space multiple-scattering calculation and interpretation of x-ray-absorption near-edge structure. *Physical Review B - Condensed Matter and Materials Physics*, *58*(12), 7565–7576. https://doi.org/10.1103/PhysRevB.58.7565

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