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Stenotrophomonas bentonitica: Formation of trigonal  
selenium nanorods and methylated species**

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## SUPPLEMENTARY MATERIAL

# **Combined bioreduction and volatilization of Se<sup>VI</sup> 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  $\lambda$ -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,  $\Delta E_0$ , was varied as a global parameter in the fits. The absorption threshold  $E_0$  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  $\text{\AA}^{-1}$  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  $\sigma_2$  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

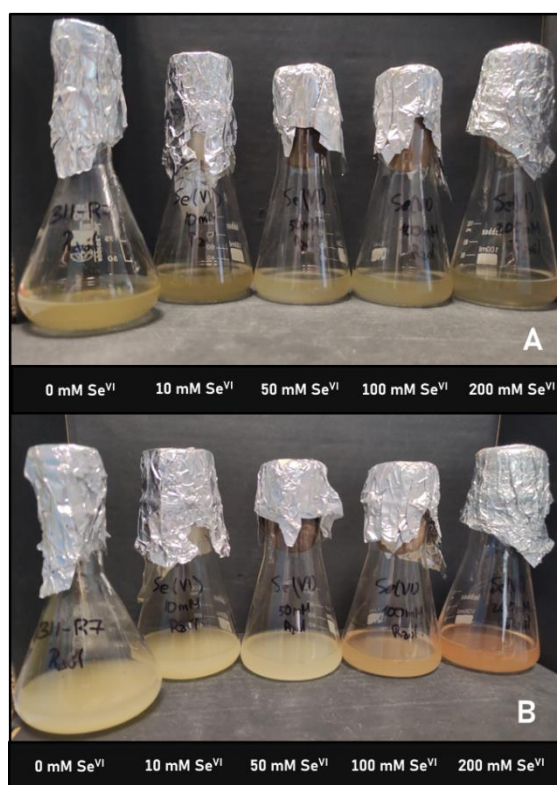


Figure S1. Cultures of *S. bentonitica* in LB broth supplemented with 0, 10, 50, 100, and 200 mM Se(VI) after 0 (A) and 48 hours (B).

Figure S2

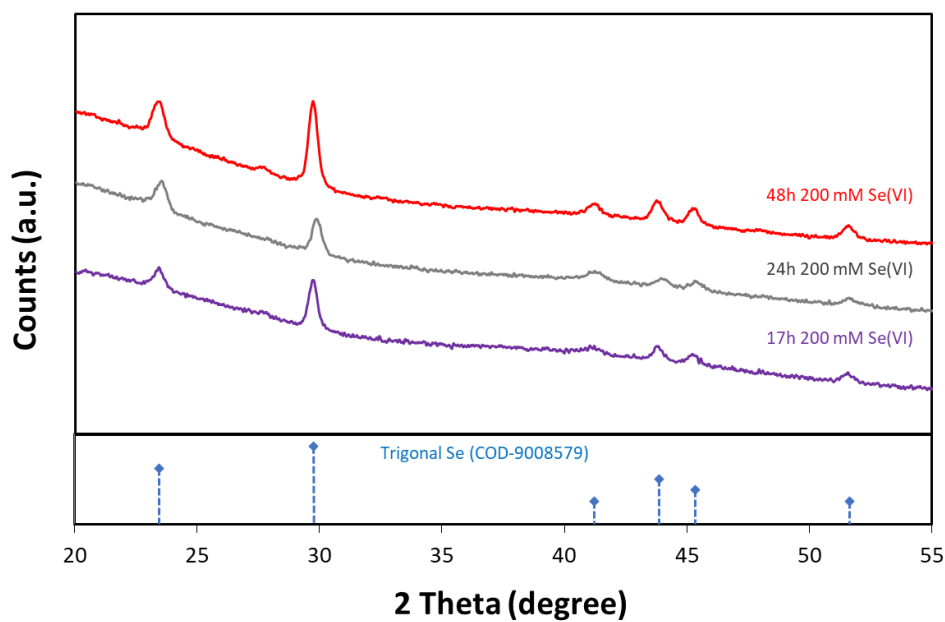
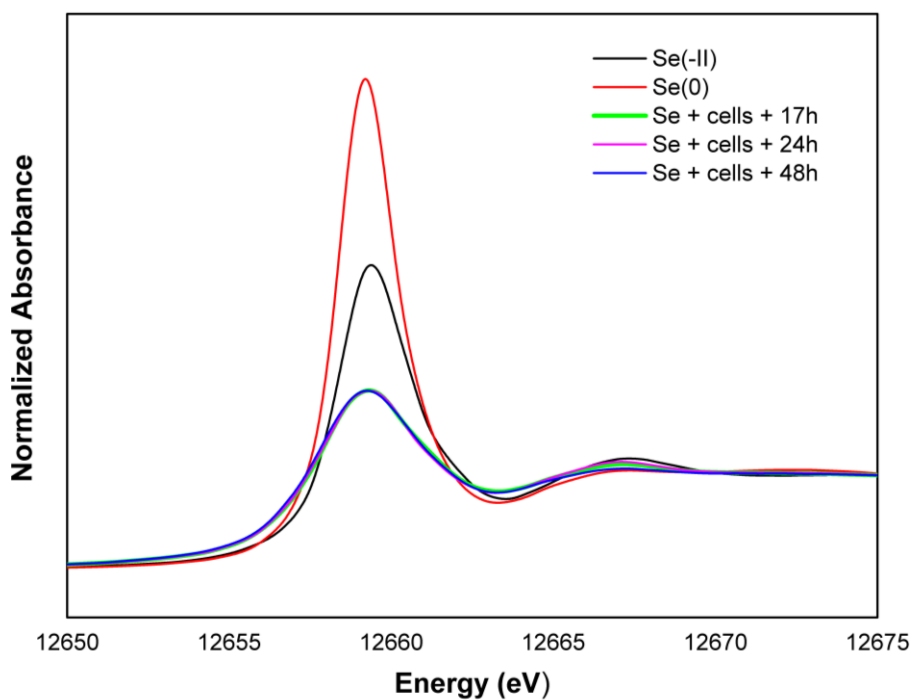


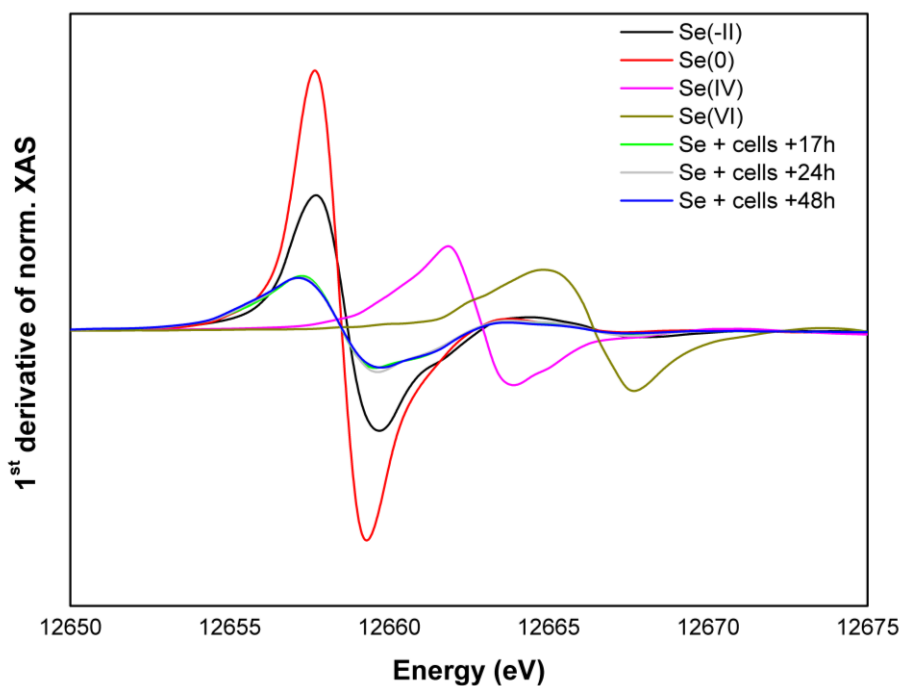
Figure S2. X-ray diffraction pattern of cultures of *S. bentonitica* supplemented with 200 mM Se(VI) after 17, 24, and 48h of incubation. Peaks for Se with a trigonal structure t-Se were detected as indicated as the corresponding peaks for t-Se (COD-9008579) obtained from Crystallography Open Database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

**Figure S3**



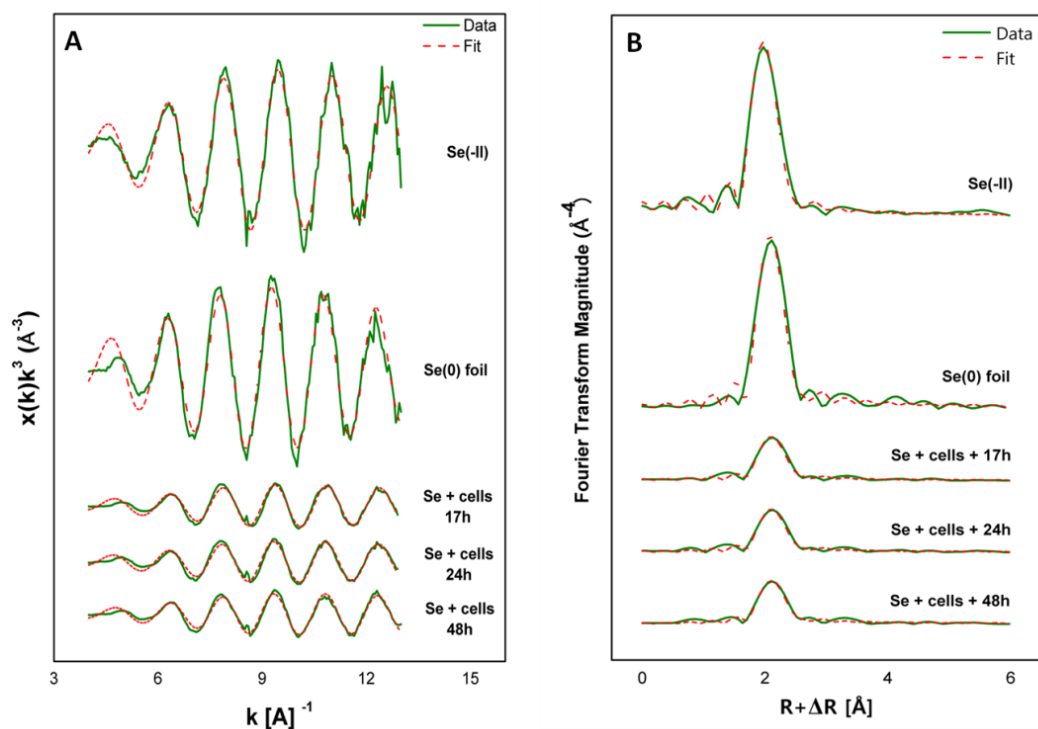
**Figure S3.** XANES spectra of Se(0) and Se(-II) references and the Se products samples after 17, 24, and 48h.

**Figure S4**



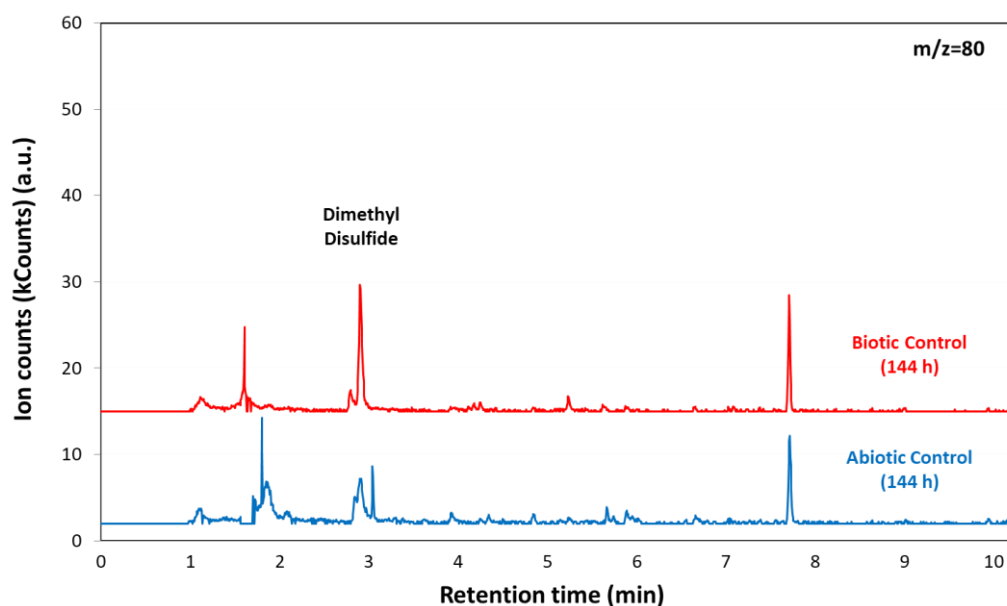
**Figure S4.** First derivative of the XANES spectra of Se reference compounds (A) and biogenic SeNPs samples produced by *S. bentonitica* at different incubation times (24, 72, and 144 h)

**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>

Solari, P. L., Schlutig, S., Hermange, H., & Sitaud, B. (2009). MARS, a new beamline for radioactive matter studies at SOLEIL. *Journal of Physics: Conference Series*, 190. <https://doi.org/10.1088/1742-6596/190/1/012042>