Supporting Information

Identification of Volatile/Semi-Volatile Products Derived from Chemical Remediation of cis-1,3-Dichloropropene by Thiosulfate

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Supporting Information: Soil Properties and Bunte Salt Synthesis

Soil Properties

Most soil experiments were conducted in an Arlington sandy loam soil (coarse-loamy, mixed, thermic Haplic Durixeralf) collected from the University of California Agricultural Experiment Station in Riverside. Other soils used in the study were Hanford sand (coarse-loamy, mixed, superactive, thermic Typic Xerorthent; Fresno, CA), Sesame sandy loam (fine-loamy, mixed, thermic Typic Haploxerolls; Paso Robles, CA), and Milham sandy loam (fine-loamy, mixed, superactive, thermic Typic Haplargids, Buttonwillow, CA). The organic carbon contents of the Arlington sandy loam, Hanford sand, Sesame sandy loam, and Milham sandy loam were 0.92%, 0.33%, 1.42%, and 1.83%, respectively, and the pH values were 7.2, 7.5, 5.7, and 7.8, respectively.

Bunte Salt Synthesis

The preparation and purification of the reaction product of cis-1,3-D and sodium thiosulfate were performed according to a modified method regarding Bunte salt synthesis. Briefly, equimolar quantities of cis-1,3-D and sodium thiosulfate were reacted at 45 °C for 5 d. The reaction solution was dried under vacuum at temperature below 55 °C. The reaction product (Bunte salt) was extracted with hot ethanol and then recrystallized in ice. The crystallization was repeated one more time. The salt was dissolved in deionized water and dried under high vacuum at room temperature to remove possible residual ethanol from the crystallization step. The product was stored at -20 °C until used.
Figure S-1. Example selected ion chromatograms of hydrolysis products of thiosulfate derivative of *cis*-1,3-D (R-S₂O₃⁻) in pH=10 and 2.0 M HCl aqueous solutions incubated at 25 °C for 1 d (Note: without the addition of internal standard in the sketch).
Figure S-2. Mass spectra (EI) of dialkyl disulfide (R-S-S-R) and mercaptan (R-SH) obtained from the hydrolysis of the thiosulfate derivative of cis-1,3-D (R-S₂O₃⁻).
Figure S-3. Time course of transformation of cis-1,3-D (0.5 mmol kg\(^{-1}\)) in Arlington sandy loam amended with thiosulfate fertilizer. (A) The dissipation of cis-1,3-D in the amended and unamended soils; (B) The production and dissipation of four identified organic sulfur products in the amended soil: the concentration of each product is normalized to the initial concentration of cis-1,3-D (0.5 mmol kg\(^{-1}\)). Error bars represent standard deviation of triplicate samples.
Figure S-4. Mass spectra (EI) of mercaptomethyl-substituted derivative (R-S-CH₃) and a disulfur-substituted methyl derivative (R-S-S-CH₃) obtained from transformation of the thiosulfate derivative of cis-1,3-D (R-S₂O₃⁻) in soil.
Figure S-5. Formation of R-S-S-R and R-S-CH$_3$ from the conversion of R-S$_2$O$_3^-$ (0.5 mmol kg$^{-1}$) in sterile and non-sterile soils. The concentrations are normalized to the initial concentration of R-S$_2$O$_3^-$ (0.5 mmol kg$^{-1}$). Error bars represent standard deviations of triplicate samples.