

1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16

Supplementary Information (SI)

for

**Mechanistic insights into extracellular reductive dechlorination of
hexachloroethane by common non-electroactive bacteria *Bacillus
subtilis* and *Escherichia coli***

Sadiq Naveed^a, Xinwei Zhou^b, and Dongqiang Zhu^{a, *}

^a Key Laboratory of the Ministry of Education for Earth Surface Processes, College of
Urban and Environmental Sciences, Peking University, Beijing 100871, China

^b College of Environmental and Chemical engineering, Jiangsu University of Science and
Technology, Jiangsu, 212003, P.R. China

*Corresponding author. Tel.: +86 010-6276-6405. E-mail: zhud@pku.edu.cn (D. Zhu)

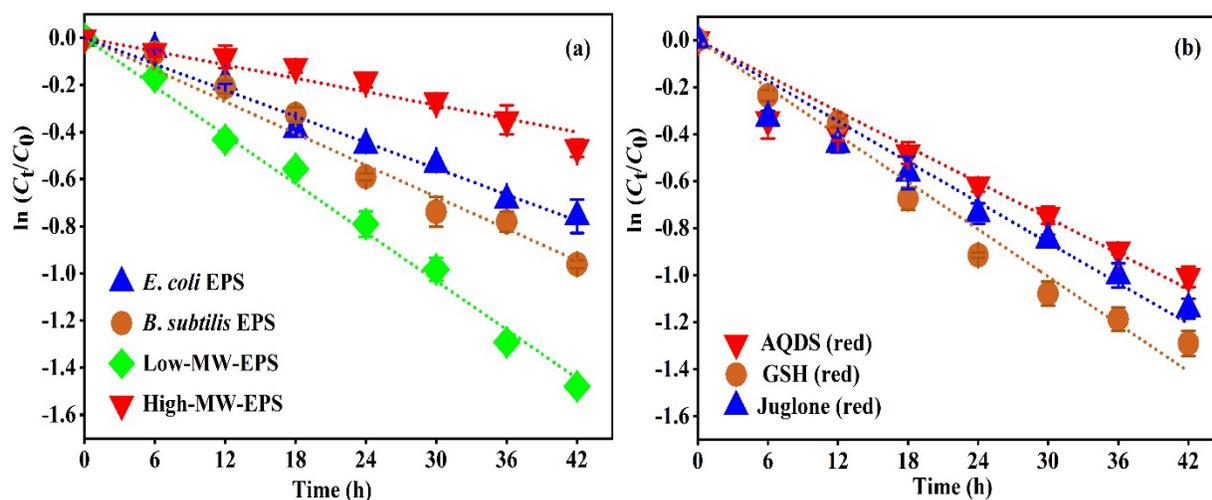
17 **Contents:**

18 **Section I. Pseudo-first-order reaction kinetics of hexachloroethane reduction by**
19 **different EPS and reducing model compounds.**

20 **Section II. One electron reduction potentials of different organic compounds.**

21

22 **Section I.**



23

24 **Fig. S1.** Pseudo-first-order reaction kinetics plotted as $\ln(C_t/C_0)$ vs. time (0-42 h) for
25 reduction of HCE at pH 7.0 and 30 °C in the dark by bulk EPS from *B. subtilis* and *E. coli*
26 (initially at 50 mg C/L) and fractional EPS from *B. subtilis* (low-MW EPS initially at 28.9
27 mg C/L; high-MW EPS initially at 18.2 mg C/L) (a) and in aqueous solutions of model
28 compounds (reduced AQDS initially at 2 mM; reduced GSH initially at 2 mM; reduced
29 juglone initially at 25 μ M) (b). Reaction conditions: 20 μ M HCE at pH 7.0 and 30 °C in
30 the dark. Error bars represent standard deviations of three replicates.

31 **Section II.**

32 **Table S1. One-electron reduction potentials (E°_1 , V) of different organic compounds**

33 **versus standard hydrogen potential (SHE) at pH 7.0.**

Compounds	E°_1 (V)	References
Hexachloroethane (HCE)	0.144	[1, 2]
Pentachlorethane (PCE)	0.092	[1]
Tetrachloroethylene (TCE)	-0.598	[2]
Nitrobenzene	-0.486	[3]
1, 3 dinitrobenzene (1,3-DNB)	-0.345	[3, 4]
Glutathione (GSH)	-0.250	[5]
Anthraquinone-2,6-disulfonic acid (AQDS)	-0.250	[6]
Juglone	-0.093	[7]

34

35 **References:**

- 36 [1] Cwiertny, D. M., Scherer, M. M., 2010. Abiotic Processes affecting the remediation of
37 chlorinated solvents. In situ remediation of chlorinated solvent plumes, 69-108. Springer, New
38 York, NY. <https://doi.org/10.1007/978-1-4419-1401-9-4>.
- 39 [2] Totten, L. A., Roberts, A. L., 2001. Calculated one-and two-electron reduction potentials and
40 related molecular descriptors for reduction of alkyl and vinyl halides in water. Crit Rev
41 Environ Sci Technol 31(2), 175-221. <https://doi.org/10.1080/20016491089208>.
- 42 [3] Neta, P., Simic, M., Hoffman, M., 1976. Pulse radiolysis and electron spin resonance
43 studies of nitroaromatic radical anions. Optical absorption spectra, kinetics, and one-
44 electron redox potentials. J Phys Chem A 80, 2018-2023.
45 <https://doi.org/10.1021/j100559a014>.
- 46 [4] Salter-Blanc, A.J., Bylaska, E.J., Johnston, H.J., Tratnyek, P.G., 2015. Predicting
47 reduction rates of energetic nitroaromatic compounds using calculated one-electron
48 reduction potentials. Environ Sci Technol 49, 3778-3786.
49 <https://doi.org/10.1021/es505092s>.
- 50 [5] Veine, D.M., Arscott, L.D., Williams, C.H., 1998. Redox Potentials for Yeast,
51 Escherichia coli and Human Glutathione Reductase Relative to the NAD⁺/NADH
52 Redox Couple: Enzyme Forms Active in Catalysis. Biochemistry 37, 15575-15582.
53 <https://doi.org/10.1021/bi9811314>.
- 54 [6] Aulenta, F., Di Maio, V., Ferri, T., Majone, M., 2010. The humic acid analogue
55 anthraquinone-2, 6-disulfonate (AQDS) serves as an electron shuttle in the electricity-

56 driven microbial dechlorination of trichloroethene to cis-dichloroethene.
57 *Bioresour Technol* 101, 9728-9733. <https://doi.org/10.1016/j.biortech.2010.07.090>.

58 [7] Mukherjee, T., 1987. One-electron reduction of juglone (5-hydroxy-1, 4-
59 naphthoquinone): a pulse radiolysis study. *Radiat Phys Chem* 29, 455-462.
60 [https://doi.org/10.1016/1359-0197\(87\)90024-5](https://doi.org/10.1016/1359-0197(87)90024-5).