Effects of cationic surfactant on the bioaccumulation of polycyclic aromatic

hydrocarbons in rice and the soil microbial community structure

Ni Ni^{a,b}, Fang Wang^a, Yang Song^{a,*}, Renyong Shi^{a,b}, Mingyun Jia^a, Yongrong Bian^a,

Xin Jiang^a

^a Key Laboratory of Soil Environment and Pollution Remediation, Institute of Soil

Science, Chinese Academy of Sciences, Nanjing 210008, PR China

^b University of the Chinese Academy of Sciences, Beijing 100049, PR China

*Corresponding authors: Tel: +86881193; Fax: +86 25 86881000, E-mail:

ysong@issas.ac.cn, Address: NO. 71 East Beijing Road, Nanjing, 210008, PR China.

Submitted to *RSC Advances*

Content

Supplemental Results

3 tables, 7 figures

		Total	Environmental	
Group	Compounds	concentrations	quality standards	
Group	compounds	(ug/kg dry soil)	(ug/kg dry soil)	
2 rings	Nanhthalene	$\frac{(\mu g) Rg (ar y (501))}{118 + 5}$	<u>(µg/kg ul/ 5011)</u> 100	
2 11155	Acenanhthene	110 ± 3 40 ± 2	500	
	Aconaphthylono	40 ± 2 27 ± 4	500	
2 min		27 ± 4	500	
3 rings	Fluorene	43 ± 2	500	
	Phenanthrene	259 ± 6	500	
	Anthracene	49 ± 4	500	
Sum of 3-rings PAHs		417 ± 12		
	Fluoranthene	909 ± 25	500	
4 rings	Pyrene	736 ± 18	500	
	Benzo[a]anthracene	691 ± 21	100	
	Chrysene	672 ± 17	100	
Sum of 4-rings PAHs		3008 ± 53		
	Benzo(b)fluoranthene	885 ± 25	100	
5 rings	Benzo(k)fluoranthene	598 ± 27	200	
	Benzo(a)pyrene	792 ± 35	100	
Sum of 5-rings PAHs		2274 ± 65		
	Indeno(1,2,3-c,d)pyrene	744 ± 54	100	
6 rings	Dibenzo(a,h)anthracene	181 ± 15	100	
	Benzo(g,h,i)perylene	739 ± 38	500	
Sum of 6-rings PAHs		1664 ± 68		
$\sum 16$ PAHs		7481 ± 105		

Table S1 Polycyclic aromatic hydrocarbon (PAH) concentrations in the soil used in this study.

The environmental quality standards refer to the two orders of magnitude of the PAH concentrations in farmland soils in China (GB 15618-2008). Means \pm standard deviation (N = 3).



Fig. S1 Dry biomass of rice after 150 days of growth. Control: no cetyltrimethylammonium bromide (CTMAB) addition; 50 CTMAB: 50 mg/kg CTMAB addition; 150 CTMAB: 150 mg/kg CTMAB addition. Different lowercase (root) and capital (shoot) letters indicate significant differences among the treatments based on LSD post hoc comparison tests at p < 0.05. Error bars indicate the standard deviation (N = 3).

	pН	Cation exchange	Organic	Dissolved organic	Nitrate	Ammonium
		capacity	matter	carbon	nitrogen	nitrogen
		(cmol/kg)	(g/kg)	(mg/kg)	(mg/kg)	(mg/kg)
Control	$7.38\pm0.02\ ab$	$14.58\pm0.30\ c$	$20.02\pm0.07\ ab$	$302 \pm 12 \text{ ab}$	51.26 ± 0.30 a	$31.52\pm0.50\ b$
50 CTMAB	$7.40 \pm 0.06 \text{ ab}$	$14.72 \pm 0.15 \text{ c}$	$20.72\pm0.24\ ab$	$289 \pm 7 ab$	51.06 ± 1.46 a	$35.12\pm1.08\ b$
150 CTMAB	$7.49\pm0.05\ a$	$14.84 \pm 0.15 \ c$	$21.34\pm0.82\ a$	312 ± 18 a	52.67 ± 0.05 a	66.91 ± 2.66 a

Table S2 Physicochemical characteristics of the soil after 150 days of rice growth.

Control: no cetyltrimethylammonium bromide (CTMAB) addition; 50 CTMAB: 50 mg/kg CTMAB addition; 150 CTMAB: 150 mg/kg CTMAB addition. Mean values with the same letter in a column are not significantly different among treatments based on LSD post hoc comparison tests at the 5% level. Means \pm standard deviation (N = 3).



Fig. S2 Concentrations of PAHs in rice grown in soils amended with/without cetyltrimethylammonium bromide (CTMAB). Control: no CTMAB addition; 50 CTMAB: 50 mg/kg CTMAB addition; 150 CTMAB: 150 mg/kg CTMAB addition. Different lowercase (root) and capital (stem, leaf and grain) letters indicate significant differences among the treatments based on LSD post hoc comparison tests at p < 0.05. Error bars indicate the standard deviation (N = 3).

	Root-shoot translocation factor	BCF _{Shoot}	BCF _{Root}	BCF _{Grain}
Control	0.125 ± 0.021 a	0.0065 ± 0.0006 a	0.0686 ± 0.0023 a	0.0021 ± 0.0003 a
50 CTMAB	0.122 ± 0.018 a	0.0065 ± 0.0009 a	0.0682 ± 0.0013 a	0.0020 ± 0.0001 a
150 CTMAB	0.124 ± 0.013 a	0.0059 ± 0.0005 a	0.0629 ± 0.0009 b	0.0019 ± 0.0001 a

 Table S3 Bioconcentration factors of carrot shoots and roots in the different treatments.

Control: no cetyltrimethylammonium bromide (CTMAB) addition; 50 CTMAB: 50 mg/kg CTMAB addition; 150 CTMAB: 150 mg/kg CTMAB addition. Mean values with the same letter in a column are not significantly different among treatments based on LSD post hoc comparison tests at the 5% level. Means \pm standard deviation (N = 3).



Fig. S3 Time course of the total concentrations of $\sum 16$ PAHs (A), 2(+3)-ring (B), 4ring (C), and 5(+6)-ring (D) PAHs in the soils after 150 days of rice growth. Control: no cetyltrimethylammonium bromide (CTMAB) addition; 50 CTMAB: 50 mg/kg CTMAB addition; 150 CTMAB: 150 mg/kg CTMAB addition. Different letters indicate significant differences among the treatments based on LSD post hoc comparison tests at *p* < 0.05. Error bars indicate the standard deviation (*N*=3).



Fig. S4 Time course of the HPCD-extracted concentrations of $\sum 16$ (A), 2(+3)-ring (B), 4-ring (C), and 5(+6)-ring (D) PAHs in the soils after 150 days of rice growth. Control: no cetyltrimethylammonium bromide (CTMAB) addition; 50 CTMAB: 50 mg/kg CTMAB addition; 150 CTMAB: 150 mg/kg CTMAB addition. Different letters indicate significant differences among the treatments based on LSD post hoc comparison tests at p < 0.05. Error bars indicate the standard deviation (N = 3).



Fig. S5 Correlations between the bioaccumulated concentrations in rice roots and the bioavailable concentrations of $\sum 16$ PAHs (A), 2(+3)-ring (B), 4-ring (C), and 5(+6)-ring (D) PAHs in the soil amended with/without cetyltrimethylammonium bromide. Error bars indicate the standard deviation (N = 3).



Fig. S6 Species richness and bacterial diversity respectively expressed as chao1 and Shannon indexes in the soils after 150 days of rice growth. Control: no cetyltrimethylammonium bromide (CTMAB) addition; 50 CTMAB: 50 mg/kg CTMAB addition; 150 CTMAB: 150 mg/kg CTMAB addition. Different lowercase (Shannon) and capital letters (chao1) indicate significant differences among the treatments by LSD post-hoc comparison tests at p < 0.05. Error bars indicate the standard deviation (N = 3).



Fig. S7 Amplification/reduction in relative abundances of bacterial phyla in the 50 cetyltrimethylammonium bromide (CTMAB) treatment (A), and that in the 150 CTMAB treatment (B) compared to the control. Error bars indicate the standard deviation (N = 3).