

SUPPLEMENTARY MATERIAL

Particle Size Distributions of PCDD/Fs and PBDD/Fs in Ambient Air in a Suburban Area in Beijing, China

Xian Zhang¹, Qing-Qing Zhu¹, Shu-Jun Dong¹, Hong-Xing Zhang², Xiao-Ke Wang², Mei Wang¹, Li-Rong Gao¹, Ming-Hui Zheng^{1}*

¹ *State Key Laboratory of Environmental Chemistry and Ecotoxicology, Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences, Beijing 100085, China*

² *Beijing Urban Ecosystem Research Station, Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences, 100085 Beijing, China*

Contents

Table S1 PCDD/F congener concentrations (fg m⁻³) in the ambient air samples.

Table S2 PBDD/F congener concentrations (fg m⁻³) in the ambient air samples.

Table S3 The monitored traces of 2,3,7,8-sbstituted PBDD/F congeners by the HRMS.

* Corresponding author. Tel.: +86-10-6284-9172; Fax: +86-10-6284-9172.

E-mail address: zhengmh@rcees.ac.cn

Supporting Information

Table S1 PCDD/F congener concentrations (fg m⁻³) in the ambient air samples.

	HD-1					HD-2					HD-3				
	a	b	c	d	e	a	b	c	d	e	a	b	c	d	e
2,3,7,8-TeCDF	23.7	4.4	0.2	0.0	19.5	27.9	2.9	2.3	3.3	51.1	11.4	4.1	2.1	1.3	60.9
1,2,3,7,8-PeCDF	59.6	8.4	1.1	0.1	27.5	51.6	9.5	7.0	0.8	30.4	29.3	8.0	3.7	0.8	38.1
2,3,4,7,8-PeCDF	107.8	11.9	1.3	0.1	4.5	91.8	7.2	5.3	3.9	22.3	45.0	12.7	6.1	1.4	28.2
1,2,3,4,7,8-HxCDF	152.3	19.5	1.0	0.4	1.6	112.0	18.7	10.2	5.0	7.6	74.3	18.7	7.5	4.0	8.7
1,2,3,6,7,8-HxCDF	118.4	16.0	1.0	0.2	0.6	104.8	16.7	8.9	4.2	6.9	72.6	18.2	7.4	3.9	8.9
2,3,4,6,7,8-HxCDF	147.4	17.5	1.4	0.4	0.8	148.9	25.5	9.2	4.6	4.1	105.8	24.1	9.1	5.3	3.9
1,2,3,7,8,9-HxCDF	39.8	5.3	0.9	0.8	1.6	33.5	5.7	2.9	1.5	0.6	22.6	4.4	2.1	0.4	0.6
1,2,3,4,6,7,8-HpCDF	552.5	65.2	6.2	1.8	1.2	477.4	69.0	29.4	14.7	4.0	341.1	74.9	27.2	12.8	4.1
1,2,3,4,7,8,9-HpCDF	81.1	10.2	0.7	0.1	0.5	72.9	10.7	4.8	1.1	0.4	55.9	13.2	4.4	0.5	0.6
OCDF	576.0	51.4	5.6	2.7	3.6	389.2	59.9	22.5	16.9	0.0	284.5	65.6	26.2	12.6	7.6
2,3,7,8-TeCDD	2.6	0.9	0.5	0.1	1.3	1.6	1.6	2.8	0.5	4.6	1.1	0.5	0.9	1.1	3.6
1,2,3,7,8-PeCDD	15.7	1.8	0.2	0.2	0.2	7.7	8.7	3.8	0.6	3.3	6.0	2.3	0.8	1.2	4.4
1,2,3,4,7,8-HxCDD	16.1	2.0	0.4	0.2	0.1	14.2	2.9	1.2	0.6	0.9	9.9	2.8	1.1	0.5	0.8
1,2,3,6,7,8-HxCDD	32.4	3.7	0.8	0.1	0.2	36.4	3.1	2.5	1.0	0.8	23.4	5.4	2.5	1.1	0.9
1,2,3,7,8,9-HxCDD	22.7	2.9	0.4	0.1	0.5	25.4	4.1	2.6	1.4	0.9	20.0	5.6	1.9	0.8	0.6
1,2,3,4,6,7,8-HpCDD	156.8	20.1	2.0	0.4	0.3	186.2	29.9	13.8	4.8	2.3	120.9	29.9	11.9	6.8	1.3
OCDD	225.5	26.6	2.5	0.8	1.7	308.1	53.3	33.5	10.9	1.2	173.0	64.8	46.3	35.2	2.9
∑2,3,7,8-PCDD/Fs			2698					2799					2179		
I-TEQ	131.3	16.3	2.1	0.5	7.6	112.3	19.3	12.2	5.2	26.4	67.6	18.1	8.5	4.4	30.4
Total I-TEQ			157.8					175.4					129.0		

	HD-4					HD-5				
	a	b	c	d	e	a	b	c	d	e
2,3,7,8-TeCDF	16.9	4.1	1.5	1.6	60.8	3.8	0.8	0.5	0.4	48.8
1,2,3,7,8-PeCDF	0.8	7.6	0.8	3.7	61.8	17.8	3.2	2.5	1.7	80.8
2,3,4,7,8-PeCDF	48.5	7.3	2.3	2.6	38.8	13.9	1.6	1.5	1.5	54.3
1,2,3,4,7,8-HxCDF	117.7	14.2	7.9	4.9	20.1	26.8	4.9	3.1	1.6	48.1
1,2,3,6,7,8-HxCDF	106.1	14.8	7.6	3.6	17.9	27.7	5.1	3.0	1.5	44.2
2,3,4,6,7,8-HxCDF	160.5	19.4	10.1	4.3	7.8	46.7	7.7	3.9	2.9	27.1
1,2,3,7,8,9-HxCDF	50.3	3.7	0.5	0.5	0.5	9.5	1.9	1.0	0.5	4.3
1,2,3,4,6,7,8-HpCDF	560.6	59.8	23.3	11.7	5.9	208.9	26.8	12.4	8.3	25.7
1,2,3,4,7,8,9-HpCDF	97.9	8.9	4.5	0.5	0.8	64.6	4.9	1.6	1.6	1.7
OCDF	494.9	46.3	16.2	10.2	4.0	238.0	33.0	17.2	18.1	8.2
2,3,7,8-TeCDD	6.4	2.1	3.4	0.5	5.8	1.1	0.1	0.1	1.3	3.0
1,2,3,7,8-PeCDD	10.5	3.2	1.9	0.5	5.2	2.4	0.3	0.2	1.2	10.0
1,2,3,4,7,8-HxCDD	12.1	1.2	1.2	0.3	3.3	2.8	0.5	0.4	0.2	2.9
1,2,3,6,7,8-HxCDD	17.9	11.6	2.3	1.2	1.9	8.1	1.7	1.0	0.9	5.1
1,2,3,7,8,9-HxCDD	5.0	3.7	1.5	1.3	0.3	6.3	1.2	1.0	0.3	3.1
1,2,3,4,6,7,8-HpCDD	164.4	23.3	7.2	4.2	1.6	68.9	10.3	5.3	4.4	3.8
OCDD	214.6	28.2	15.6	5.0	1.5	131.5	19.2	11.1	10.6	3.8
Σ2,3,7,8-PCDD/Fs			2747					1499		
I-TEQ	93.5	16.0	9.2	4.2	42.3	27.1	4.0	2.7	3.7	57.9
Total I-TEQ			165.2					95.4		

a. $d_{ae} < 1.0 \mu\text{m}$; b. $d_{ae} 1.0\text{--}2.5 \mu\text{m}$; c. $d_{ae} 2.5\text{--}10 \mu\text{m}$; d. $d_{ae} > 10 \mu\text{m}$; e. gas phase.

Abbreviations: tetra = Te; penta = Pe; hexa = Hx; hepta = Hp; and octa = O ; international toxic equivalent quantity= I-TEQ

Table S2 PBDD/F congener concentrations (fg m⁻³) in the ambient air samples.

	HD-1					HD-2					HD-3				
	a	b	c	d	e	a	b	c	d	e	a	b	c	d	e
2,3,7,8-TeBDD	1.9	5.2	0.1	1.0	0.9	1.7	4.2	0.3	1.0	0.9	2.3	1.6	1.3	2.6	2.3
1,2,3,7,8-PeBDD	3.3	3.3	1.1	0.5	0.4	2.8	2.7	1.1	0.6	0.6	5.6	1.0	1.6	1.1	3.0
1,2,3,4,7,8- HxBDD															
1,2,3,6,7,8-HxBDD	2.6	12.5	1.2	2.5	1.6	2.2	9.8	1.2	2.1	1.4	7.1	3.8	6.9	3.3	8.8
1,2,3,7,8,9-HxBDD	3.8	5.6	1.2	3.3	3.4	3.2	4.5	1.1	2.8	2.8	7.6	5.8	3.6	5.3	3.9
1,2,3,4,6,7,8-HpBDD	10.9	8.2	14.4	5.4	10.3	8.6	6.6	11.3	4.4	8.1	21.0	11.1	3.8	5.7	17.8
OBDD	61.8	13.5	55.4	21.4	9.1	47.7	10.6	42.8	16.7	7.2	40.9	23.3	37.0	13.8	36.4
2,3,7,8-TeBDF	24.8	5.2	7.0	3.3	7.6	19.3	4.3	5.6	2.7	6.1	28.0	5.7	3.2	1.7	3.5
1,2,3,7,8-PeBDF	20.5	5.4	3.6	3.8	4.0	15.9	4.4	3.0	3.2	3.3	20.9	9.5	3.9	2.5	3.8
2,3,4,7,8-PeBDF	17.2	4.5	0.8	1.2	0.6	13.5	3.7	0.8	1.1	0.7	42.3	4.5	4.3	2.3	4.3
1,2,3,4,7,8-HxBDF	60.5	12.1	7.9	3.4	2.5	46.7	9.5	6.3	2.8	2.2	96.1	13.8	7.4	4.3	3.3
1,2,3,4,6,7,8-HpBDF	448.5	100.7	71.2	46.2	23.6	345.0	77.6	54.9	35.8	18.4	417.1	145.9	62.7	35.8	8.0
OBDF	197.0	58.4	33.5	31.4	33.2	151.6	45.1	26.0	24.4	25.7	157.2	50.9	41.7	42.9	244.1
∑2,3,7,8-PBDD/Fs			1505					1171					1761		
TEQ	24.8	14.6	4.2	3.8	3.5	19.7	11.9	3.8	3.5	3.3	39.5	8.8	7.1	6.4	9.0
Total TEQ			50.9					42.2					70.8		

	HD-4					HD-5				
	a	b	c	d	e	a	b	c	d	e
2,3,7,8-TeBDD	2.8	0.5	0.4	1.2	0.2	0.9	0.9	1.8	0.6	0.3
1,2,3,7,8-PeBDD	3.2	1.0	1.4	1.8	0.6	3.2	0.7	1.5	1.6	0.7
1,2,3,4,7,8- HxBDD	5.6	5.3	4.4	3.2	2.6	2.8	1.5	7.2	8.1	4.9
1,2,3,6,7,8-HxBDD										
1,2,3,7,8,9-HxBDD	3.3	2.7	1.4	6.4	1.9	2.9	2.2	2.9	8.8	9.3
1,2,3,4,6,7,8-HpBD	18.0	6.0	4.1	5.9	8.5	5.4	11.8	6.3	3.0	16.1
OBDD	5.7	4.2	7.9	2.9	10.0	8.1	2.4	3.4	6.3	10.9
2,3,7,8-TeBDF	82.8	4.8	6.3	3.4	3.7	44.1	6.7	2.6	1.9	60.8
1,2,3,7,8-PeBDF	27.1	3.3	4.6	4.2	1.4	56.3	4.1	2.1	3.4	8.9
2,3,4,7,8-PeBDF	79.4	3.2	4.8	1.7	1.3	23.9	2.6	3.7	2.8	2.4
1,2,3,4,7,8-HxBDF	275.3	10.3	11.8	9.4	1.4	125.	8.4	4.2	5.8	2.8
1,2,3,4,6,7,8-HpBD	895.7	75.1	72.4	34.9	11.1	439.	89.2	41.8	14.5	16.2
OBDF	342.8	81.6	67.5	25.6	36.2	137.	97.6	14.7	52.0	32.8
∑2,3,7,8-PBDD/Fs			2424					1445		
TEQ	88.2	5.7	6.6	6.3	2.4	35.0	5.5	6.7	5.8	10.2
Total TEQ			109.3					63.1		

a. $d_{ae} < 1.0 \mu\text{m}$; b. $d_{ae} 1.0\text{--}2.5 \mu\text{m}$; c. $d_{ae} 2.5\text{--}10 \mu\text{m}$; d. $d_{ae} > 10 \mu\text{m}$; e. gas phase.

Abbreviations: tetra = Te; penta = Pe; hexa = Hx; hepta = Hp; and octa = O; toxic equivalent quantity= TE

Table S3 The monitored traces of 2,3,7,8-substituted PBDD/F congeners by the HRMS.

Window	homologs	M/Z	M/Z type	Compounds
1	Br-4	480.96966	Lock mass	PFK
		481.69740	M+2	TeBDF
		483.69540	M+4	TeBDF
		493.73770	M+2	¹³ C-TeBDF
		495.73570	M+4	¹³ C-TeBDF
		497.69230	M+2	TeBDD
		499.69030	M+4	TeBDD
		504.96966	Cali mass	PFK
		511.73060	M+4	¹³ C-TeBDD
		513.72860	M+6	¹³ C-TeBDD
		2	Br-5	554.96650
561.60590	M+4			PeBDF
563.60390	M+6			PeBDF
573.64620	M+4			13C- PeBDF
575.64420	M+6			13C- PeBDF
577.60080	M+4			PeBDD
579.59880	M+6			PeBDD
589.64110	M+4			13C- PeBDD
591.63910	M+6			13C- PeBDD
592.96327	Cali mass			PFK
3	Br-6			604.96327
		639.51640	M+4	HxBDF
		641.51440	M+6	HxBDF
		651.55660	M+4	13C-HxBDF
		653.55460	M+6	13C-HxBDF
		654.96008	Cali mass	PFK

		655.51130	M+4	HxBDD
		657.50930	M+6	HxBDD
		667.55150	M+4	¹³ C- HxBDD
		669.54950	M+6	¹³ C- HxBDD
4	Br-7	692.95690	Lock mass	PFK
		719.42480	M+6	HpBDF
		721.42280	M+8	HpBDF
		731.46510	M+6	¹³ C- HpBDF
		733.46310	M+8	¹³ C- HpBDF
		735.41980	M+6	HpBDD
		737.41780	M+8	HpBDD
		742.95366	Cali mass	PFK
		747.46000	M+6	¹³ C-HpBDD
		749.45800	M+8	¹³ C-HpBDD
5	Br-8	730.95369	Lock mass	PFK
		797.33530	M+6	OBDF
		799.33330	M+8	OBDF
		804.95050	Cali mass	PFK
		809.37560	M+6	¹³ C- OBDF
		811.37360	M+8	¹³ C- OBDF
		813.33020	M+6	OBDD
		815.32820	M+8	OBDD
		825.37050	M+6	¹³ C-OBDD
		827.36850	M+8	¹³ C-OBDD
