Supporting Information (3 figures and 3 tables)

Occurrence and profiles of chlorinated and brominated polycyclic aromatic hydrocarbons in waste incinerators

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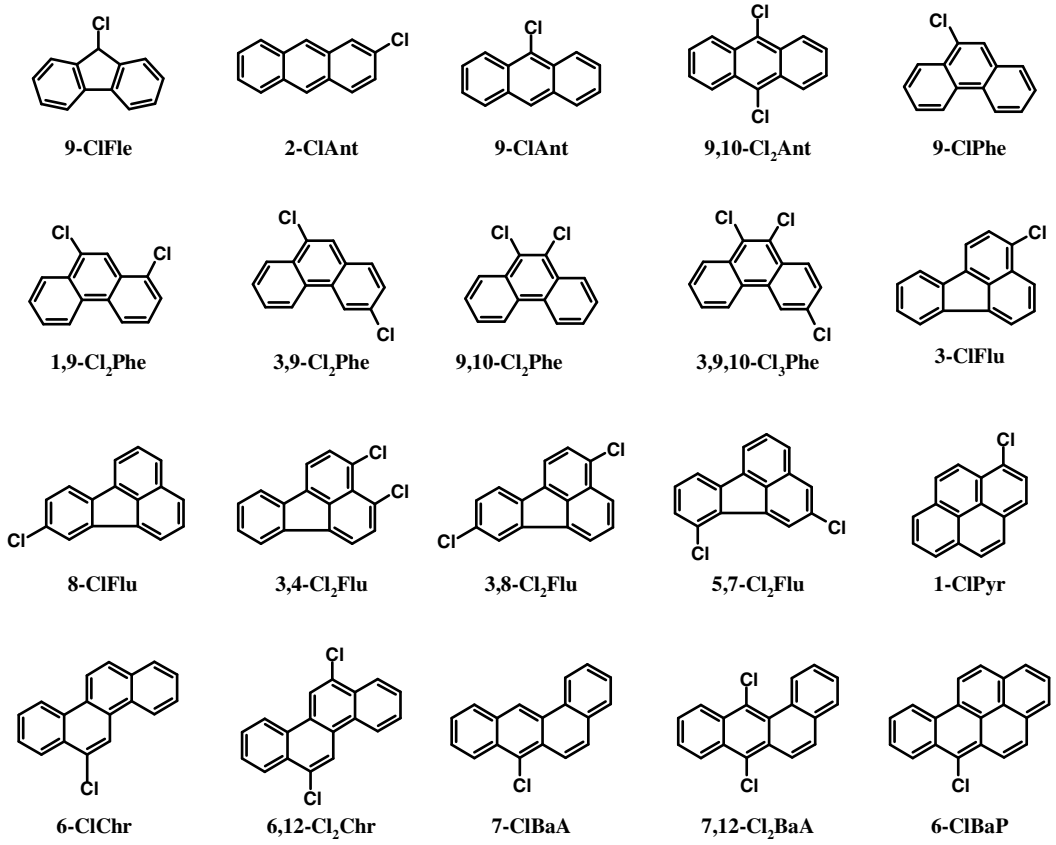

Figure S1. Chemical structures of 20 chlorinated PAHs analyzed.

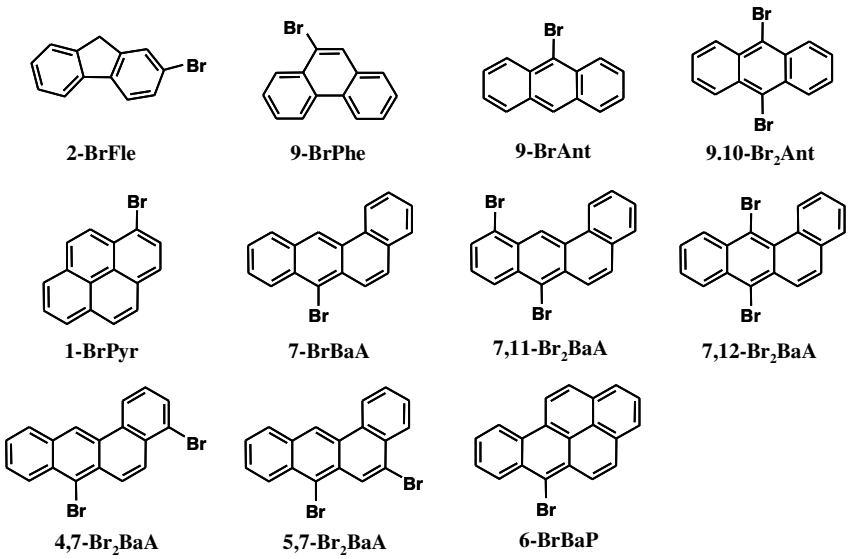

Figure S2. Chemical structures of 11 brominated PAHs analyzed.

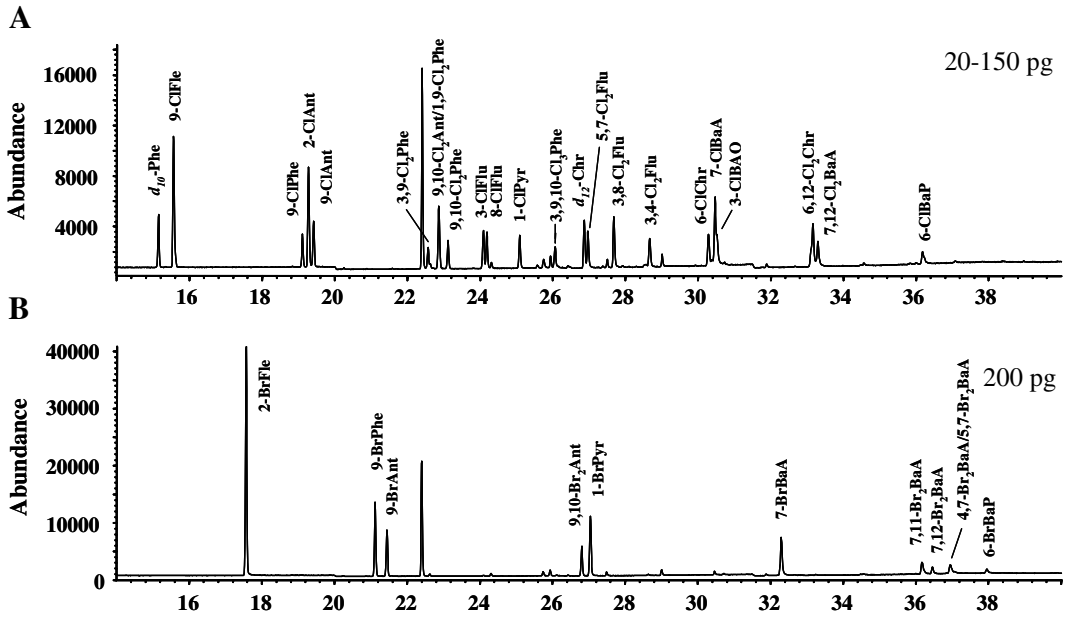

Figure S3. Mass chromatograms of 20 chlorinated PAH standards (A) and 11 brominated PAH standards (B).

Table S1. Details of incinerator types studied.

ID	type	capacity (kg/h)	outlet temp. (°C)	waste type
I1	fixed grate	95	910	municipal
I2	stoker	8330	980	municipal
I3	rotary kiln	190	860	hazardous
I4	fixed grate	350	840	municipal/ industrial
I5	fixed grate	1000	950	municipal
I6	fixed grate	1000	880	municipal
I7	fixed grate	100	680	hazardous
I8	fixed grate	120	680	municipal/ industrial
I9	fixed grate	95	980	municipal
I10	fixed grate	500	970	municipal
I11	stoker	12500	960	municipal

Table S2. List of target compounds along with their abbreviations, ion monitored, limit of quantification; LOQ (ng/g), and AhR- potency values relative to benzo[a]pyrene.

compound	abbrev.	ions monitored	LOQ (ng/g)	AhR-mediated activity REP_{BaP} [a]	Recovery (%) n=3
chlorinated polycyclic aromatic hydrocarbons	**ClPAHs**				
9-monochlorofluorene	**9-ClFle**	200, 202, 165	0.06		103
9-monochlorophenanthrene	**9-ClPhe**	212, 214	0.06	0.03	112
2-monochloroanthracene	**2-ClAnt**	212, 214	0.06	0.1	104
9-monochloroanthracene	**9-ClAnt**	212, 214	0.06	0.03	93
3,9-dichlorophenanthrene	**3,9-Cl2Phe**	246, 248	0.06	0.32	113
9,10-dichloroanthracene [b]	**9,10-Cl_2Ant**	246, 248	0.06	0.2	107
1,9-dichlorophenanthrene [b]	**1,9-Cl_2Phe**	246, 248	0.06	0.12	107
9,10-dichlorophenanthrene	**9,10-Cl_2Phe**	246, 248	0.06	0.16	114
3-monochlorofluoranthene	**3-ClFlu**	236, 238	0.06	0.17	114
8-monochlorofluoranthene	**8-ClFlu**	236, 238	0.06	0.18	118
1-monochloropyrene	**1-ClPyr**	236, 238	0.06	0.1	114
3,9,10-trichlorophenanthrene	**3,9,10-Cl_3Phe**	280, 282	0.14	0.77	114
5,7-dichlorofluoranthene	**5,7-Cl_2Flu**	270, 272	0.06		115
3,8-dichlorofluoranthene	**3,8-Cl_2Flu**	270, 272	0.06	5.7	106
3,4-dichlorofluoranthene	**3,4-Cl_2Flu**	270, 272	0.06		102
6-chlorochrysene	**6-ClChr**	262, 264	0.06	2.1	115
7-chlorobenz[a]anthracene	**7-ClBaA**	262, 264	0.06	0.83	109
6,12-dichlorochrysene	**6,12-Cl_2Chr**	296, 298	0.14	0.03	120
7,12-dichlorobenz[a]anthracene	**7,12-Cl_2BaA**	296, 298	0.14	0.1	109
6-monochlorobenzo[a]pyrene	**6-Cl-BaP**	286, 288	0.14	0.09	108
brominated polycyclic aromatic hydrocarbons	**BrPAHs**				
2-monobromofluorene	**2-BrFle**	244, 246, 165	0.14		98
9-monobromophenanthrene	**9-BrPhe**	256, 258	0.14		105
9-monobromoanthracene	**9-BrAnt**	256, 258	0.14		91
9,10-dibromoanthracene	**9,10-Br_2Ant**	336, 334	0.14		97
1-monobromopyrene	**1-BrPyr**	280, 282	0.14		97
7-monobromobenz[a]anthracene	**7-BrBaA**	306, 308	0.14		113
7,11-dibromobenz[a]anthracene	**7,11-Br_2BaA**	386, 384	0.29		120
7,12-dibromobenz[a]anthracene	**7,12-Br_2BaA**	386, 384	0.29		72
4,7-dibromobenz[a]anthracene [b]	**4,7-Br_2BaA**	386, 384	0.29		112
5,7-dibromobenz[a]anthracene [b]	**5,7-Br_2BaA**	386, 384	0.29		112
6-monobromobenzo[a]pyrene	**6-BrBaP**	300, 332	0.29		107
polycyclic aromatic hydrocarbons	**PAHs**				
naphthalene	**Nap**	128, 127	5.8		
acenaphthylene	**Acl**	152, 151	0.38		
acenaphthene	**Ace**	153, 154	0.38		
fluorene	**Fle**	166, 165	2.8		
phenanthrene	**Phe**	178, 176	9.9		
anthracene	**Ant**	178, 176	0.25		
fluoranthene	**Flu**	202, 200	2.40		

pyrene	**Pyr**	202, 200	0.86	
benz[*a*]anthracene	**BaA**	228, 226	0.06	
chrysene	**Chr**	228, 226	0.20	
benzo[*b*]fluoranthene	**BbF**	252, 250	0.07	
benzo[*k*]fluoranthene	**BkF**	252, 250	0.12	
benzo[*a*]pyrene	**BaP**	252, 250	0.04	
indeno[*1,2,3-cd*]pyrene	**IDP**	276, 277	0.14	
dibenz[*a,h*]anthracene	**DBahA**	278, 276	0.14	
benzo[*g,h,i*]perylene	**BghiP**	276, 277	0.14	
d_8-naphthalene	**d_8-Nap**	136, 135		60
d_{10}-acenaphthene	**d_{10}-Ace**	163, 164		88
d_{10}-phenanthrene	**d_{10}-Phe**	188, 186		107
d_{12}-chrysene	**d_{12}-Chr**	240, 238		104
d_{12}-perylene	**d_{12}-Per**	264, 260		95

[a] EC_{50} potencies for ClPAHs relative to BaP reported by Ohura et al. (2007)

[b] Compounds coelute in this study

Table S3. Ranges of concentrations (ng/g) for individual chlorinated PAHs (ClPAHs), brominated PAHs (BrPAHs), and PAHs in fly ash and bottom ash.

compound	fly ash	bottom ash
ClPAHs		
9-ClFle	LOQ (<0.06)	LOQ (<0.06)
9-ClPhe	<0.06 - 237	<0.06 - 16
2-ClAnt	<0.06 - 15	<0.06 - 0.68
9-ClAnt	<0.06 - 231	<0.06 - 1.0
3,9-Cl2Phe	<0.06 - 46	<0.06 - 3.1
9,10-Cl2Ant/ 1,9-Cl2Phe	<0.06 - 276	<0.06 - 8.8
9,10-Cl2Phe	<0.06 - 17	<0.06 - 8.6
3-ClFlu	<0.06 - 1015	<0.06 - 4.0
8-ClFlu	<0.06 - 107	<0.06 - 1.1
1-ClPyr	<0.06 - 1113	<0.06 - 2.6
3,9,10-Cl3Phe	<0.14 - 706	<0.14 - 3.4
5,7-Cl2Flu	<0.06 - 8.7	<0.06 - 1.1
3,8-Cl2Flu	<0.06 - 410	<0.06 - 2.9
3,4-Cl2Flu	<0.06 - 131	<0.06 - 0.76
6-ClChr	<0.06 - 1156	<0.06 - 7.9
7-ClBaA	<0.06 - 874	<0.06 - 0.92
6,12-Cl2Chr	<0.14 - 867	<0.14 - 2.5
7,12-Cl2BaA	<0.14 - 1133	<0.14 - 2.9
6-ClBaP	<0.14 - 5290	<0.14 - 0.68
ΣClPAHs	<0.06 - 6992	<0.06 - 68
BrPAHs		
2-BrFle	LOQ (<0.14)	LOQ (<0.14)
9-BrPhe	<0.14 - 133	<0.14 - 0.25
9-BrAnt	<0.14 - 19	<0.14 - 0.65
9,10-Br2Ant	<0.14 - 2.0	LOQ (<0.14)
1-BrPyr	<0.14 - 758	LOQ (<0.14)
7-BrBaA	<0.14 - 181	LOQ (<0.14)
7,11-Br2BaA	LOQ (<0.29)	LOQ (<0.29)
7,12-Br2BaA	<0.29 - 147	LOQ (<0.29)
4,7-/ 5,7-Br2BaA	<0.29 - 6.8	LOQ (<0.29)
6-BrBaP	<0.29 - 243	LOQ (<0.29)
ΣBrPAHs	<0.14 - 1235	<0.14 - 0.65
PAHs		
Nap	<5.8 - 5184	<5.8 - 793
Acl	<0.38 - 7252	<0.38 - 29
Ace	<0.38 - 55	<0.38 - 12
Fle	<2.8 - 57	<2.8 - 42
Phe	<9.9 - 59267	<9.9 - 297
Ant	<0.25 - 5104	<0.50 - 57
Flu	<2.4 - 45324	<2.4 - 86
Pyr	<0.86 - 54874	3.6 - 109
BaA	<0.06 - 8957	<0.06 - 38
Chr	<0.2 - 15461	<0.2 - 94

BbF	<0.07 - 9933	<0.07 - 31
BkF	<0.12 - 10472	<0.12 - 16
BaP	<0.04 - 5625	<0.04 - 11
IDP	<0.14 - 7042	<0.14 - 16
DBahA	<0.14 - 687	<0.14 - 17
BghiP	<0.14 - 11399	<0.14 - 26
ΣPAHs	2.4 - 244830	9.1 - 1531

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