TABLE II Resulting main PCDF fragments from the chlorophenols by pyrolysis at 400C

Fragment in resulting PCDF	used Phenol by H-Elimination	Phenol by C-Elimination
0	Phenol	2-C-Phenol
1	3- C-Phenol	2,3-C-Phenol
2	4- C-Phenol	2,4-C-Phenol
3	3- C-Phenol	2,5-C-Phenol
4	2- C-Phenol	2,6-C-Phenol
12	3,4- C-Phenol	2,3,4-C-Phenol
13	3,5- C-Phenol	2,3,5-C-Phenol
14	2,5- C-Phenol	2,3,6-C-Phenol
23	3,4- C-Phenol	2,4,5-C-Phenol
24	2,4- C-Phenol	2,4,6-C-Phenol
34	2,3- C-Phenol	2,3,6-C-Phenol
123	3,4,5- C-Phenol	2,3,4,5-C-Phenol
124	2,4,5- C-Phenol	2,3,4,6-C-Phenol
134	2,3,5- C-Phenol	2,3,5,6-C-Phenol
234	2,3,4- C-Phenol	2,3,4,6-C-Phenol
1234	2,3,4,5- C-Phenol	2,3,4,5,6-C-Phenol

TABLE III Sources of the PCDDs and PCDFs with 1 to 3 chlorines

No.	Isomer	CA registry number	Sources and purity
MCDDs			
1	1	39227-53-7	(a)AccuStandard Inc., U.S.A. ; 100%(GC/MS) (b) Pyrolysis(P+23-DiCP);
2	2	39227-54-8	(a)AccuStandard Inc., U.S.A. ; 100%(GC/MS) (b)Cambridge Isotope Lab., USA; (c) Pyrolysis(P+24-DiCP);
DiCDDs			
1	12		Pyrolysis(2-CP+234-TrCP);
2	13		Pyrolysis(2-CP+246-TrCP);
3	14		Pyrolysis(2-CP+236-TrCP);
4	16		Pyrolysis(23-DiCP);
5	17		Pyrolysis(23-DiCP+24-DiCP);
6	18		Pyrolysis(23-DiCP+24-DiCP);
7	19		Pyrolysis(23-DiCP);
8	23	29446-15-9	(a)AccuStandard Inc., U.S.A. ; 100%(GC/MS) (b)Cambridge Isotope Lab., USA;
9	27	33857-26-0	(a)AccuStandard Inc., U.S.A. ; 100%(GC/MS) (b) Pyrolysis(24-DiCP)
10	28	38964-22-6	(a)Wellington Lab., U.S.A. ; > 98%(GC/MS) (b) Pyrolysis(24-DiCP)
TrCDDs			
1	123	54536-17-3	(a)AccuStandard Inc., U.S.A. ; 100%(GC/MS) (b) Pyrolysis(2-CP+2345-TeCP)
2	124	39227-58-2	(a)AccuStandard Inc., U.S.A. ; 100%(GC/MS) (b)Copyrolysis(2356-TeCP+2-CP)
3	126		Pyrolysis(23-DiCP+234-TrCP)
4	127		Pyrolysis(24-DiCP+234-TrCP)
5	128		Pyrolysis(24-DiCP+234-TrCP)
6	129		Pyrolysis(23-DiCP+234-TrCP)
7	136		Pyrolysis(23-DiCP+246-TrCP)
8	137	67028-17-5	Pyrolysis(24-DiCP+246-TrCP)
9	138		Pyrolysis(24-DiCP+246-TrCP)
10	139		Pyrolysis(23-DiCP+246-TrCP)
11	146		Pyrolysis(23-DiCP+236-TrCP)
12	147		Pyrolysis(24-DiCP+236-TrCP)
13	178		Pyrolysis(23-DiCP+245-TrCP)
14	237	33857-28-2	(a)AccuStandard Inc., U.S.A. ; 100%(GC/MS) (b) Cambridge Isotope Lab., USA; (c)Pyrolysis(24-DiCP+245-TrCP)

Acronyms [a] CDD = chlorinated dibenzo-p-dioxins ; CDF = chlorinated dibenzofurans ; CP = chlorophenols; M= mono; Di = di; Tr = tri;

TABLE III*(continued)* Sources of the PCDDs and PCDFs with 1 to 3 chlorines

No.	Isomer	CA registry number	Sources and purity
MCDFs			
1	1		(a) J. Ogaki ; (b) Pyrolysis(P+3-CP)
2	2	43047-99-0	(a) Wellington Lab., U.S.A. ; > 98%(GC/MS) (b) Cambridge Isotope Lab., USA; (c) Pyrolysis(P+4-CP)

3	3		(a) Pyrolysis(P+3-CP)
4	4		(a) Wellington Lab., U.S.A. ; > 98%(GC/MS)
			(b) Pyrolysis(P+2-CP)
DiCDFs			
1	12		Pyrolysis(P+34-DiCP)
2	13		Pyrolysis(P+35-DiCP)
3	14		Pyrolysis(P+25-DiCP)
4	16		Pyrolysis(3-CP+2-CP)
5	17		Pyrolysis(3-CP)
6	18		Pyrolysis(3-CP+4-CP)
7	19		Pyrolysis(3-CP)
8	23		(a)Wellington Lab., U.S.A. ; > 98%(GC/MS)
			(b)Pyrolysis(P+34-DiCP)
9	24		(a) Pyrolysis(P+24-DiCP)
10	26		(a)Wellington Lab., U.S.A. ; > 98%(GC/MS)
			(b) Pyrolysis(4-CP+2-CP)
11	27		(a) Wellington Lab., U.S.A. ; > 99%(GC/MS)
			(b) Pyrolysis(4-CP+3-CP)
12	28	5409-83-6	(a) Wellington Lab., U.S.A. ; 97%(GC/MS)
			(b) Cambridge Isotope Lab., USA;
			(c) Pyrolysis(4-CP); (NMR)
13	34		(a)J.Ogaki
			(b) Pyrolysis(P+23-DCP)
14	36		(a)J.Ogaki
			(b) Pyrolysis(3-CP+2-CP)
15	37		Pyrolysis(3-CP)
16	46		(a) Pyrolysis(2-CP); oxygen:CP= 1:1
			(b) J.Ogaki
TrCDFs			
1	123		Pyrolysis(P+345-TrCP)
2	124		Pyrolysis(P+245-TrCP)
3	126		Pyrolysis(34-DiCP+2-CP)
4	127		Pyrolysis(34-DiCP+3-CP)
5	128		Pyrolysis(34-DiCP+4-CP)
6	129		Pyrolysis(34-DiCP+3-CP)
7	134		Pyrolysis(P+235-TrCP)
8	136		(a) Wellington Lab., U.S.A. ; > 98%(GC/MS)
			(b) Pyrolysis(35-DiCP+2-CP);
9	137		Pyrolysis(35-DiCP+3-CP)
10	138		(a)Wellington Lab., U.S.A. ; > 98%(GC/MS)
			(b) Pyrolysis(35-DiCP+4-CP)
11	139		Pyrolysis(35-DiCP+3-CP)
12	146		(a)Wellington Lab., U.S.A. ; > 98%(GC/MS)
			(b) Pyrolysis(25-DiCP+2-CP)
13	147		Pyrolysis(25-DiCP+3-CP)
14	148		Pyrolysis(25-DiCP+4-CP)
15	149		(a)Wellington Lab., U.S.A. ; > 98%(GC/MS)
			(b) Pyrolysis(25-DiCP+3-CP)
16	167		(a) via
			(b) Pyrolysis(23-DiCP+3-CP)
17	168		Pyrolysis(24-DiCP+3-CP)
18	178		Pyrolysis(34-DiCP+3-CP)
19	234		(a) Pyrolysis(P+234-TrCP)
20	236		(a)Wellington Lab., U.S.A. ; > 98%(GC/MS)
			(b) Pyrolysis(34-DiCP+2-CP)
21	237		Pyrolysis(34-DiCP+3-CP)
22	238		(a)Wellington Lab., U.S.A. ; > 98%(GC/MS)
			(b)Pyrolysis(34-DiCP+4-CP)
23	246		(a)Wellington Lab., U.S.A. ; > 98%(GC/MS)
			(b)Pyrolysis(24-DiCP+2-CP)
24	247		(a)Wellington Lab., U.S.A. ; > 98%(GC/MS)
			(b)Pyrolysis(24-DiCP+3-CP)
25	248		Pyrolysis(24-DiCP, 4-CP) ;
26	267		(a)Wellington Lab., U.S.A. ; > 98%(GC/MS)
			(b)Pyrolysis(23-DiCP, 4-CP)
27	346		(a)J.Ogaki
			(b) Pyrolysis(23-DiCP, 2-CP)
28	347		Pyrolysis(23-DiCP+3-CP)

Acronyms [a] CDD = chlorinated dibenzo-p-dioxins ; CDF = chlorinated dibenzofurans ; CP = chlorophenols; M= mono; Di = di; Tr = tri;

TABLE IV Monitoring ion for hrgc/hrms-sim mesurement

MCDF	202.0185, 204.0159;	MCDD	218.0135, 220.0108
DiCDF	235.9796, 237.9768;	DiCDD	251.9745, 253.9717
TrCDF	269.9406, 271.9377;	TrCDD	285.9355, 287.9327
TeCDF	303.9016, 305.8987;	TeCDD	319.8965, 321.8936

^{13}C-2-MCDF	214.0588;	^{13}C-2-MCDD 230.0537
^{13}C-28-DiCDF	248.0198;	^{13}C-23-DiCDD 264.0147
^{13}C-248-TrCDF	281.9809;	^{13}C-237-TrCDD 297.9758

Lock Mass 242.9856 PFP (PerFluoroPhenanthrene)

TABLE V GC silicone fused-silica capillary columns used for separation of PCDDs , PCDFs and PCBs and their temperature programs

Name	Manufacturer	Coating and type	Length	ID	Film thickness
SP-2331	Supelco , USA	biscyanopropyl(90%) Phenyl cyanopropyl 1;1 (10%) wall coated , stabilized	30m	0.25mm	0.20um
	Temperature program	120 (1min)to 200℃ (30℃/min) to 260℃(2℃/min)			

TABLE VI GC retention times of PCDD/PCDF isomers relative to RT reference standard on a SP-2331 fused-silica capillary columns

Elution	order	Isomer	RRT	Elution	order	Isomer	RRT
MCDD					11	36	1.367
	1	2	1.000		12	28	1.379
	2	1	1.070		13	26	1.416
DiCDD					14	19	1.431
	1	13	1.000		15	34	1.445
	2	27	1.083		16	46	1.508
	3	23	1.083	TrCDF			
	4	28	1.083		1	137	1.000
	5	14	1.135		2	138	1.051
	6	17	1.135		3	136	1.067
	7	18	1.150		4	168	1.099
	8	16	1.197		5	134	1.107
	9	12	1.220		6	124	1.138
	10	19	1.283		7	147	1.138
TrCDD					8	178	1.199
	1	137	1.000		9	148	1.212
	2	138	1.007		10	123	1.231
	3	136	1.037		11	139	1.247
	4	124	1.070		12	127	1.247
	5	139	1.094		13	146	1.252
	6	237	1.111		14	167	1.266
	7	147	1.122		15	247	1.291
	8	123	1.148		16	128	1.305
	9	178	1.167		17	126	1.324
	10	127	1.216		18	248	1.343
	11	128	1.232		19	246	1.385
	12	146	1.243		20	237	1.418
	13	126	1.296		21	149	1.418
	14	129	1.387		22	234	1.480
MCDF					23	238	1.480
	1	1	1.000		24	347	1.501
	2	3	1.073		25	236	1.501
	3	2	1.114		26	267	1.544
	4	4	1.182		27	129	1.595
DiCDF					28	346	1.612
	1	13	1.000		-	1368-TeCDF	1.214
	2	17	1.104		-	1368-TeCDD	1.288
	3	14	1.156				
	4	18	1.173				
	5	16	1.208				
	6	12	1.241				
	7	24	1.241				
	8	37	1.269				
	9	27	1.312				
	10	23	1.343				

2-MCDD=1.001, 13-DiCDD=1.177, 137-TrCDD=1.506, 1368-TeCDF=1.756
13-DiCDF=1.098, 137-TrCDF=1.363, 1368-TeCDF=1.654 (1-MCDF=1.000)