CONTAINS NO CBI

HERCULES

Medical Department

24-PP

Hercules Incorporated
Hercules Plaza
Wilmington, DE 19894-0001
(302) 594-5000
Telex: 4994538

July 27, 1992

8EHQ-0792-2747 SUPP

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Dear Coordinator:

TSCA 8(e) NOTICE:
8EHQ-0392-2747

Attached is a revised public version of the subject 8(e) notice. I hope you will find this satisfactory. If you have any questions, please don't hesitate to call. Ms. Lewis also can give you additional background on this revised version.

Sincerely,

Richard S. Waritz, Ph.D.
Manager, Toxicology
302/594-7059

RSW/elm
tsca8e

cc: Ms. C. Lewis, USEPA

HERCULES

Medical Department

Hercules Incorporated
Hercules Plaza
Wilmington, DE 19894-0001
(302) 594-5000
Telex: 4994538

January 30, 1992

RETURN RECEIPT REQUESTED

Document Processing Center
(Attention: Section 8(e) Coordinator)
OTS/USEPA
401 M Street, SW
Washington, DC 20460

Dear Coordinator:

TSCA 8(e) NOTICE 8EHQ-0392-2747

This information is being submitted under the provisions of the Toxic Substances Control Act, 90 Stat. 2029, 15 USC 2607, Section 8(e). Some of the information is Confidential Business Information (CBI) and is so identified. A nonconfidential version is attached. The answers to the usual six CBI questions are attached.

Also attached are 1) a copy of a report we have received on the chlorinated dibenzo-p-dioxin (dioxin) and chlorinated dibenzofuran content of i) a precursor to an R&D chemical Hercules has been evaluating and ii) combustion products from composites containing the R&D chemical [Attachment A], and 2) a spreadsheet [Attachment B] which reorganizes the pyrolysis data into a more systematic presentation. All analyses were by EPA Method 1613. The chemical structures of both the precursor and the R&D chemical are shown in Attachment C. Compound 2, the R&D chemical being developed by Hercules for . Compound 1 is the precursor.

As you can see in Attachments A and B, trace amounts of chlorinated dioxins and chlorinated dibenzofurans were present in Compound 1 as it is currently made. As also shown, when composite containing Compound 2 is incinerated at 800°C in air, lesser amounts of chlorinated dioxins and dibenzofurans are formed than from the "household refuse" standard.

Typical composites containing Compound 2 would be expected to contain approximately Compound 1. Their ITEF (International Toxicity Equivalency

Factor relative to 2,3,78-tetrachlorodioxin [TCDD]) is calculated to be 0.09 ng/kg, or 90 ppq. By comparison, the FDA's ADI for TCDD in fish fillets is 25,000 ppq. As you know, the official EPA method for TCDD in soil has a detection limit of 300,000 ppq. Concentrations ≤ than this number are reported to be zero. Also, 1,000,000 ppq of TCDD is acceptable in residential soil. Thus, the amounts found in Compound 1 and composites are trivial from a toxicological standpoint.

The dioxin and dibenzofuran levels may be even more trivial than it now appears. In calculating the ITEF from the results of analyses carried out by EPA Method 1613, the ITEF values for the more toxic isomers are calculated individually. The concentrations of the other isomers are pooled and the ITEF calculated for the pool. However, the report from the test laboratory suggests they may have calculated an ITEF for the sum of all isomers at each level of chlorination and added this to the ITEF for the more toxic isomers with that level of chlorination. This is suggested by their use of the work "summe" rather than "ohne" in the tables of analytical values. This procedure would double the contribution of the more toxic isomers to the calculated ITEF for each level of chlorination. They have not yet responded to our inquiries regarding their calculation methodology. We will forward their response when we receive it.

R&D quantities of Compound 1 and of Compound 2 are being made and used at the Hercules Research Center. in the U.S. to date has been at the Hercules Research Center. When commercial, would be sold containing Compound 2. This is calculated to have an ITEF of 180 ppq.

We do not believe that either Compound 1 or Compound 2 fall under the EPA Dioxin Rule, 40 CFR 766. Nevertheless, we will carry out a quality control program on the production of both. It will be disclosed fully in our PMN to be filed shortly.

We also recognize that Compound 1 can form a chlorinated dioxin in its own right. The two possible structures are shown in Attachment D. When attempted to prepare both isomers for Hercules for toxicological studies, they could only make the trans isomer (Isomer 2). The cis isomer (Isomer 1) would not form.

We have discussed the possible dioxin-like activity of Isomer 2 with Dr. A. E. Munson of the Medical College of Virginia; Dr. M. A. Gallo, Robert Wood Johnson Medical School-University of Medicine and Dentistry of New Jersey; and with Dr. J. P. Gierthy, New York State Department of Health. None of these experts believe that this chemical will bind to the Ah locus and, thus, is not expected to show any dioxin-like activity.

Nevertheless, they have agreed to carry out the following studies on Isomer 2:

1) Humoral immunotoxic effects and general immunotoxic effects - Dr. Munson

2) Ah locus binding and induction of cytochromes P450-1A1 and -1A2 in mice - Dr. Gallo

3) Effect on estrogen metabolism - Dr. Gierthy

The first and third studies are in progress. The second is scheduled to start in March. We expect all three studies to be completed this spring. Copies of the study reports will be added to the PMN file and can be added to this 8(e) file, if you request.

We plan to ask for a pre-notice communication with OPTS before filing the PMN. We will review this information with them as well as our other toxicity information and our quality assurance program at that time. A representative of your office is welcome to attend.

Sincerely,

Richard S. Waritz

Richard S. Waritz, Ph.D., DABT, DATS
Manager, Toxicology

RSW/elm
Attachments

ATTACHMENT A

(Research Center)

FAX # (302) 995-

TO: K.S. Waitz 4-7255

MAILSTOP: 2441 NE

PHONE: 4-7059

FROM: _____

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c.c. c.c. HERCULES RESEARCH.

Please find attached 2 reports ex

A). Report on "Dioxine" formation of composite containing modified 2,6-dichloro-4-t-octyl phenol (DCOP) submitted to burning trials at 400, 600 - 800 °C.
The analytical data are compared with "Haus müll" and not considered to be of serious concern in law of Dioxines

B) Report on "Dioxine" content of DCOP

2 Phenol were submitted for analysis
A. straight
B. Heat treated phenol.
The Heat treated phenol shows substantial quantities of of Dioxine.
The Phenol is typically diluted

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However in the complex preparation the phenol is being handled and possibly maltreated (overheated).
Would appreciate your comments/ view on above issue B)

Thank you in advance

c.c.

Hercules Research
Wilmington.

PRESTATEMENT 1 MEETING

SEPTEMBER 10 & 11 1991

1. Composite combustion trials

A sample of composite from a trial was send to the in Germany for model incineration trials. The program as pointed out in PRP note 1632/91 is now in the stage of quantification of possible alkylated dioxins with help of a previously synthesized reference. This work is expected to be finished by the end of September '91.

So far, combustions of the material (powdered under a nitrogen blanket) have been carried out as requested at 400, 600 and 800 °C. Ashes and burning gasses were combined and analyzed for known dioxins and dibenzofurans (see attached report). The analysis results are expressed as toxicity equivalents, which is a summation of the toxicity of the components found according to standardized toxicity increments: BGA/UBA values according to the Bundes Gesundheits Amt/Umwelt Bundes Amt regulations and I-TEF which is a NATO standard (International Toxicological Equivalent Factor). The values found for composite very reassuring as they fall in the same range as for e.g. and are significantly lower than for representative household refuse.

Unsere Auftrags-Nr.
Pr.Nr.

27. August 1991

Untersuchung auf polychlorierte Dibenzodioxine und polychlorierte Dibenzofurane

- Ihr Auftrag vom 17.05.91; Zeichen: FCM/1 99062 NN -

Sehr geehrter

entsprechend Ihrem Auftrag vom 17.05.91 haben wir die erhaltene Probe auf polychlorierte Dibenzodioxine und polychlorierte Dibenzofurane nach Verbrennung bei 400 °C, 600 °C und 800 °C untersucht. Die Asche und die Verbrennungsgase wurden vereint und die Dioxine daraus bestimmt. Gleichzeitig erhalten Sie die Gehalte von Dioxinen im Hausmüll nach Verbrennung bei 800 °C.

In der Anlage finden Sie die Analysenergebnisse Ihrer Proben.

Probeneingang: 18.06.91

Für Rückfragen stehen wir Ihnen gerne zur Verfügung.

Wir bedanken uns für Ihren Auftrag.

Mit freundlichen Grüßen

Anlage

U N T E R S U C H U N G S B E R I C H T

Anlage 1 zum Schreiben vom 27. August 1991
an:

Unsere Auftrags-Nr.
Pr.Nr.
Probenbeschreibung: Composite
Verbrennung bei 400 °C

		µg/kg
Polychlorierte Dibenzodioxine		
TCDD:	2,3,7,8-Tetrachlordibenzodioxin	[illegible]
	Summe Tetrachlordibenzodioxine (Cl_4-PCDD)	3050
PeCDD:	1,2,3,7,8-Pentachlordibenzodioxin	72
	Summe Pentachlordibenzodioxine (Cl_5-PCDD)	1700
HxCDD:	1,2,3,4,7,8-Hexachlordibenzodioxin	27
	1,2,3,6,7,8-Hexachlordibenzodioxin	10
	1,2,3,7,8,9-Hexachlordibenzodioxin	28
	Summe Hexachlordibenzodioxine (Cl_6-PCDD)	627
HpCDD:	1,2,3,4,6,7,8-Heptachlordibenzodioxin	294
	Summe Heptachlordibenzodioxine (Cl_7-PCDD)	449
OCDD:	Octachlordibenzodioxin	944
Polychlorierte Dibenzofurane		
TCDF:	2,3,7,8-Tetrachlordibenzofuran	203
	Summe Tetrachlordibenzofurane (Cl_4-PCDF)	3040
PeCDF:	Summe 1,2,3,7,8-Pentachlordibenzofuran u. 1,2,3,4,8-Pentachlordibenzofuran	46
	2,3,4,7,8-Pentachlordibenzofuran	14
	Summe Pentachlordibenzofurane (Cl_5-PCDF)	255
HxCDF:	Summe 1,2,3,4,7,8-Hexachlordibenzofuran u. 1,2,3,4,7,9-Hexachlordibenzofuran	13
	1,2,3,6,7,8-Hexachlordibenzofuran	< 10
	1,2,3,7,8,9-Hexachlordibenzofuran	< 10
	2,3,4,6,7,8-Hexachlordibenzofuran	< 10
	Summe Hexachlordibenzofurane (Cl_6-PCDF)	34
HpCDF:	1,2,3,4,6,7,8-Heptachlordibenzofuran	< 10
	1,2,3,4,7,8,9-Heptachlordibenzofuran	< 10
	Summe Heptachlordibenzofurane (Cl_7-PCDF)	< 10
OCDF:	Octachlordibenzofuran	5780
Toxizitätsäquivalente nach BGA/UBA:		
	Polychlorierte Dibenzodioxine	205
	Polychlorierte Dibenzofurane	64
	Summe	269
Toxizitätsäquivalente (nach I-TEF)		219

U N T E R S U C H U N G S B E R I C H T

Anlage 2 zum Schreiben vom 27. August 1991
an:

Unsere Auftrags-Nr.
Pr.Nr.
Probenbeschreibung: Composite
Verbrennung bei 600 °C

		ng/kg
Polychlorierte Dibenzodioxine		
TCDD:	2,3,7,8-Tetrachlordibenzodioxin	151
	Summe Tetrachlordibenzodioxine (Cl_4-PCDD)	3260
PeCDD:	1,2,3,7,8-Pentachlordibenzodioxin	63
	Summe Pentachlordibenzodioxine (Cl_5-PCDD)	1860
HxCDD:	1,2,3,4,7,8-Hexachlordibenzodioxin	36
	1,2,3,6,7,8-Hexachlordibenzodioxin	28
	1,2,3,7,8,9-Hexachlordibenzodioxin	10
	Summe Hexachlordibenzodioxine (Cl_6-PCDD)	835
HpCDD:	1,2,3,4,6,7,8-Heptachlordibenzodioxin	674
	Summe Heptachlordibenzodioxine (Cl_7-PCDD)	1100
OCDD:	Octachlordibenzodioxin	2630
Polychlorierte Dibenzofurane		
TCDF:	2,3,7,8-Tetrachlordibenzofuran	140
	Summe Tetrachlordibenzofurane (Cl_4-PCDF)	5280
PeCDF:	Summe 1,2,3,7,8-Pentachlordibenzofuran u. 1,2,3,4,8-Pentachlordibenzofuran	47
	2,3,4,7,8-Pentachlordibenzofuran	< 10
	Summe Pentachlordibenzofurane (Cl_5-PCDF)	246
HxCDF:	Summe 1,2,3,4,7,8-Hexachlordibenzofuran u. 1,2,3,4,7,9-Hexachlordibenzofuran	14
	1,2,3,6,7,8-Hexachlordibenzofuran	< 10
	1,2,3,7,8,9-Hexachlordibenzofuran	< 10
	2,3,4,6,7,8-Hexachlordibenzofuran	< 10
	Summe Hexachlordibenzofurane (Cl_6-PCDF)	132
HpCDF:	1,2,3,4,6,7,8-Heptachlordibenzofuran	60
	1,2,3,4,7,8,9-Heptachlordibenzofuran	< 10
	Summe Heptachlordibenzofurane (Cl_7-PCDF)	99
OCDF:	Octachlordibenzofuran	3060
Toxizitätsäquivalente nach BGA/UBA:		
	Polychlorierte Dibenzodioxine	231
	Polychlorierte Dibenzofurane	78
	Summe	310
Toxizitätsäquivalente (nach I-TEF)		221

U N T E R S U C H U N G S B E R I C H T

Anlage 3 zum Schreiben vom 27. August 1991
an:

Unsere Auftrags-Nr.
Pr.Nr.
Probenbeschreibung: Composite
Verbrennung bei 800 °C

Polychlorierte Dibenzodioxine		ng/kg
TCDD:	2,3,7,8-Tetrachlordibenzodioxin	48
	Summe Tetrachlordibenzodioxine (Cl_4-PCDD)	817
PeCDD:	1,2,3,7,8-Pentachlordibenzodioxin	135
	Summe Pentachlordibenzodioxine (Cl_5-PCDD)	1610
HxCDD:	1,2,3,4,7,8-Hexachlordibenzodioxin	23
	1,2,3,6,7,8-Hexachlordibenzodioxin	< 10
	1,2,3,7,8,9-Hexachlordibenzodioxin	< 10
	Summe Hexachlordibenzodioxine (Cl_6-PCDD)	514
HpCDD:	1,2,3,4,6,7,8-Heptachlordibenzodioxin	180
	Summe Heptachlordibenzodioxine (Cl_7-PCDD)	349
OCDD:	Octachlordibenzodioxin	152
Polychlorierte Dibenzofurane		
TCDF:	2,3,7,8-Tetrachlordibenzofuran	25
	Summe Tetrachlordibenzofurane (Cl_4-PCDF)	1300
PeCDF:	Summe 1,2,3,7,8-Pentachlordibenzofuran u. 1,2,3,4,8-Pentachlordibenzofuran	12
	2,3,4,7,8-Pentachlordibenzofuran	< 10
	Summe Pentachlordibenzofurane (Cl_5-PCDF)	108
HxCDF:	Summe 1,2,3,4,7,8-Hexachlordibenzofuran u. 1,2,3,4,7,9-Hexachlordibenzofuran	< 10
	1,2,3,6,7,8-Hexachlordibenzofuran	< 10
	1,2,3,7,8,9-Hexachlordibenzofuran	< 10
	2,3,4,6,7,8-Hexachlordibenzofuran	< 10
	Summe Hexachlordibenzofurane (Cl_6-PCDF)	92
HpCDF:	1,2,3,4,6,7,8-Heptachlordibenzofuran	< 10
	1,2,3,4,7,8,9-Heptachlordibenzofuran	< 10
	Summe Heptachlordibenzofurane (Cl_7-PCDF)	< 10
OCDF:	Octachlordibenzofuran	< 10
Toxizitätsäquivalente nach BGA/UBA:		
	Polychlorierte Dibenzodioxine	93
	Polychlorierte Dibenzofurane	16
	Summe	110
Toxizitätsäquivalente (nach I-TEF)		121

14

UNTERSUCHUNGSBERICHT

Repräsentativer Hausmüll

Verbrennungstemperatur: 800 °C

Polychlorierte Dibenzodioxine		ng/kg
TCDD:	2,3,7,8-Tetrachlordibenzodioxin	54,1
	Summe Tetrachlordibenzodioxine (Cl_4-PCDD)	1480
PeCDD:	1,2,3,7,8-Pentachlordibenzodioxin	136
	Summe Pentachlordibenzodioxine (Cl_5-PCDD)	1630
HxCDD:	1,2,3,4,7,8-Hexachlordibenzodioxin	84,4
	1,2,3,6,7,8-Hexachlordibenzodioxin	159
	1,2,3,7,8,9-Hexachlordibenzodioxin	103
	Summe Hexachlordibenzodioxine (Cl_6-PCDD)	1150
HpCDD:	1,2,3,4,6,7,8-Heptachlordibenzodioxin	364
	Summe Heptachlordibenzodioxine (Cl_7-PCDD)	437
OCDD:	Octachlordibenzodioxin	653

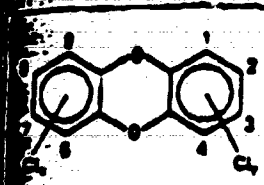
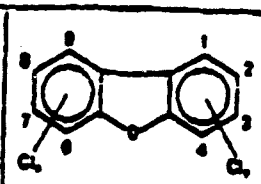
Polychlorierte Dibenzofurane		
TCDF:	2,3,7,8-Tetrachlordibenzofuran	711
	Summe Tetrachlordibenzofurane (Cl_4-PCDF)	7030
PeCDF:	Summe 1,2,3,7,8-Pentachlordibenzofuran u. 1,2,3,4,8-Pentachlordibenzofuran	305
	2,3,4,7,8-Pentachlordibenzofuran	468
	Summe Pentachlordibenzofurane (Cl_5-PCDF)	4770
HxCDF:	Summe 1,2,3,4,7,8-Hexachlordibenzofuran u. 1,2,3,4,7,9-Hexachlordibenzofuran	7[illegible],0
	1,2,3,6,7,8-Hexachlordibenzofuran	75,[illegible]
	1,2,3,7,8,9-Hexachlordibenzofuran	52,2
	2,3,4,6,7,8-Hexachlordibenzofuran	66,3
	Summe Hexachlordibenzofurane (Cl_6-PCDF)	1280
HpCDF:	1,2,3,4,6,7,8-Heptachlordibenzofuran	189
	1,2,3,4,7,8,9-Heptachlordibenzofuran	136
	Summe Heptachlordibenzofurane (Cl_7-PCDF)	538
OCDF:	Octachlordibenzofuran	622

Toxizitätsäquivalente nach BGA/HBA:		
	Polychlorierte Dibenzodioxine	144
	Polychlorierte Dibenzofurane	292
	Summe	436

Anhang

A1 Strukturen der PCDD und PCDF

Tabelle 7. Strukturen der PCDD und PCDF und Anzahl der möglichen Isomeren

	
PCDD Polychlorierte Dibenzodioxine	PCDF Polychlorierte Dibenzofurane

Anzahl der Chloratome	Anzahl der CDD-Isomeren	Anzahl der CDF-Isomeren
1	2	4
2	10	16
3	14	28
4	22	38
5	14	28
6	10	16
7	2	4
8	1	1
Summe	75	135

A2 Berechnung der Toxizitätsäquivalente

Außer der Be[illegible]ung der Toxizitätsäquivalente nach BGA/UBA gibt es eine Reihe weiterer Berechnungsverfahren von TCDD-Äquivalenten, z.B. nach EPA, Eadon, Nordische Methode (siehe Tabelle 8).

Tabelle 8. Toxizitätsäquivalente nach unterschiedlichen Berechnungsmethoden

	Eadon 86	EPA	BGA/UBA	LMS	BUS	Nordische Methode
2,3,7,8-TCDD	1	1	1	1	1	1
ohne 2,3,7,8	–	0.01	0.01	–	0.01	–
2,3,7,8-PeCDD	1	0.5	0.1	0.1	0.1	0.5
ohne 2,3,7,8	–	0.005	0.01	–	0.1	–
2,3,7,8-HxCDD	0.033	0.04	0.1	0.1–0.01	0.1	0.1
ohne 2,3,7,8	–	0.0004	0.0	–	0.1	–
2,3,7,8-HpCDD	–	0.001	0.01	0.01	0.01	0.01
ohne 2,3,7,8	–	0.00001	0.001	–	0.01	–
OCDD	–	–	0.001	–	–	0.001
2,3,7,8-TCDF	0.33	0.1	0.1	0.1	0.1	0.1
ohne 2,3,7,8	–	0.001	0.01	–	0.1	–
2,3,7,8-PeCDF	0.33	0.1	0.1	0.2–0.1	0.1	0.5–0.01 *)
ohne 2,3,7,8	–	0.001	0.01	–	0.1	–
2,3,7,8-HxCDF	0.021	0.01	0.1	0.2–0.05	0.1	0.1
ohne 2,3,7,8	–	0.0001	0.01	–	0.1	–
2,3,7,8-HpCDF	–	0.01	0.01	0.01	0.1	0.01
ohne 2,3,7,8	–	0.00001	0.001	–	0.1	–
OCDF	–	–	0.001	–	–	0.001
Σ TetraCDD **)	–	–	0.01	–	–	–
Σ PentaCDD **)	–	–	0.01	–	–	–
Σ HexaCDD **)	–	–	0.01	–	–	–
Σ HeptaCDD **)	–	–	0.001	–	–	–
Σ TetraCDF **)	–	–	0.01	–	–	–
Σ PentaCDF **)	–	–	0.01	–	–	–
Σ HexaCDF **)	–	–	0.01	–	–	–
Σ HeptaCDF **)	–	–	0.001	–	–	–

3. BERICHT

zur Bestimmung von

alkyl-substituierten polychlorierten Dibenzodioxinen

in DCOP

Dezember 1991

Blatt 2 zum 3. Bericht vom 30.12.91

zur Bestimmung von alkyl-substituierten polychlorierten Dibenzodioxinen in DCOP

Unsere Auftrags-Nr.

Folgende Proben wurden untersucht:

Probennummer	Probenbezeichnung	Identifikation GC/MS
	DCOP	
91TG082165	RG 16:091 A DCOP (usual)	Sample 1, Sample 3
91TG082166	RG 16:091 B DCOP (heated)	Sample 2, Sample 4

Die PCDD- und PCDF-Ergebnisse der beiden Proben sind durch sehr hohe Tetra- HexaCDF-Summenwerte auffallend, die wiederum aus nicht 2,3,7,8-substituierten Einzelkongeneren geprägt sind. Wie aus den beiliegenden Chromatogrammen ersichtlich ist, können diese als folgende PCDF/Kongenere identifiziert werden:

1,4,6,9-/2,4,6,8-	TCDF
2,3,6,8-	TCDF
1,2,4,6,8-	PCDF
1,3,4,7,9-/1,2,3,6,8-	PCDF
1,2,3,6,8-/2,3,4,8,9-	PCDF
1,2,3,4,6,8-	HCDF
2,3,4,6,7,8-	HCDF

Die alkylierten, polychlorierten Dibenzodioxine wurden, wie bereits in den früheren Berichten aufgelistet, auf dialkylierte, di- bis pentachlorierte Dibenzodioxine hin untersucht. Die Zuordnung Verbindungsklasse und Verbindungs-Nr. ist identisch wie im früheren Bericht.

Blatt 3 zum 3. Bericht vom 30.12.91
an:

zur Bestimmung von alkyl-substituierten polychlorierten Dibenzodioxinen in DCOP

Unsere Auftrags-Nr.

Bei den jetzt untersuchten Proben ergab sich für folgende Verbindungen eine Übereinstimmung der Isotopenverhältnisse < ± 5 % der theoretischen Werte:

Verbindungs-Nr.:	Summenformel	Alkylreste
1	$C_{28}H_{35}Cl_5O_2$	$R_1 = C_8H_{17}$ $R_2 = C_8H_{17}$
2	$C_{28}H_{37}Cl_3O_2$	$R_1 = C_8H_{17}$ $R_2 = C_8H_{17}$
6	$C_{28}H_{36}Cl_4O_2$	$R_1 = C_8H_{17}$ $R_2 = C_8H_{17}$
17	$C_{24}H_{29}Cl_3O_2$	$R_1 = C_6H_{13}$ $R_2 = C_6H_{13}$
31	$C_{22}H_{26}Cl_2O_2$	$R_1 = C_5H_{11}$ $R_2 = C_5H_{11}$

Für folgende Verbindungen ergab sich eine Übereinstimmung der Isotopenverhältnisse < ± 15 % der theoretischen Werte:

4	$C_{24}H_{28}Cl_4O_2$	$R_1 = C_6H_{13}$ $R_2 = C_6H_{13}$
12	$C_{16}H_{11}Cl_5O_2$	$R_1 = C_2H_5$ $R_2 = C_2H_5$
15	$C_{20}H_{20}Cl_4O_2$	$R_1 = C_4H_9$ $R_2 = C_4H_9$
22	$C_{15}H_{10}Cl_4O_2$	$R_2 = CH_3$ $R_2 = C_2H_5$

Bei allen anderen Massenspuren lag das Isotopenverhältnis > ± 15 % oder es konnten keine Substanzpeaks identifiziert werden.

Mit freundlichen Grüßen

U N T E R S U C H U N G S B E R I C H T

Anlage 1 zum 3. Bericht vom 30.12.91

Unsere Auftrags-Nr.
Pr.Nr.
Probenbeschreibung: 10 ml Glasflasche, BG 16 1091 A DCOP

		ng/kg
Polychlorierte Dibenzodioxine		
TCDD:	2,3,7,8-Tetrachlordibenzodioxin	34,3
	Summe Tetrachlordibenzodioxine (Cl_4-PCDD)	136
PeCDD:	1,2,3,7,8-Pentachlordibenzodioxin	2,2
	Summe Pentachlordibenzodioxine (Cl_5-PCDD)	21,8
HxCDD:	1,2,3,4,7,8-Hexachlordibenzodioxin	3,8
	1,2,3,6,7,8-Hexachlordibenzodioxin	24,3
	1,2,3,7,8,9-Hexachlordibenzodioxin	10,3
	Summe Hexachlordibenzodioxine (Cl_6-PCDD)	73,1
HpCDD:	1,2,3,4,6,7,8-Heptachlordibenzodioxin	75,4
	Summe Heptachlordibenzodioxine (Cl_7-PCDD)	85,0
OCDD:	Octachlordibenzodioxin	55,1
Polychlorierte Dibenzofurane		
TCDF:	2,3,7,8-Tetrachlordibenzofuran	11,6
	Summe Tetrachlordibenzofurane (Cl_4-PCDF)	6480
PeCDF:	Summe 1,2,3,7,8-Pentachlordibenzofuran u. 1,2,3,4,8-Pentachlordibenzofuran	60,0
	2,3,4,7,8-Pentachlordibenzofuran	7,5
	Summe Pentachlordibenzofurane (Cl_5-PCDF)	47800
HxCDF:	Summe 1,2,3,4,7,8-Hexachlordibenzofuran u. 1,2,3,4,7,9-Hexachlordibenzofuran	8,3
	1,2,3,6,7,8-Hexachlordibenzofuran	5,7
	1,2,3,7,8,9-Hexachlordibenzofuran	5,2
	2,3,4,6,7,8-Hexachlordibenzofuran	97,6
	Summe Hexachlordibenzofurane (Cl_6-PCDF)	2620
HpCDF:	1,2,3,4,6,7,8-Heptachlordibenzofuran	60,2
	1,2,3,4,7,8,9-Heptachlordibenzofuran	5,8
	Summe Heptachlordibenzofurane (Cl_7-PCDF)	89,4
OCDF:	Octachlordibenzofuran	80,7
Toxizitätsäquivalente nach BGA/UBA:		
	Polychlorierte Dibenzodioxine	40,7
	Polychlorierte Dibenzofurane	567
	Summe	608
Toxizitätsäquivalente (nach I-TEF)		60,4

U N T E R S U C H U N G S B E R I C H T

Anlage 2 zum 3. Bericht vom 30.12.91

Unsere Auftrags-Nr.
Pr.Nr.
Probenbeschreibung: 10 ml Glasflasche, RG 16 1091 B DCOP

Polychlorierte Dibenzodioxine		ng/kg
TCDD:	2,3,7,8-Tetrachlordibenzodioxin	73,0
	Summe Tetrachlordibenzodioxine (Cl_4-PCDD)	1460
PeCDD:	1,2,3,7,8-Pentachlordibenzodioxin	40,2
	Summe Pentachlordibenzodioxine (Cl_5-PCDD)	282
HxCDD:	1,2,3,4,7,8-Hexachlordibenzodioxin	16,4
	1,2,3,6,7,8-Hexachlordibenzodioxin	133
	1,2,3,7,8,9-Hexachlordibenzodioxin	118
	Summe Hexachlordibenzodioxine (Cl_6-PCDD)	451
HpCDD:	1,2,3,4,6,7,8-Heptachlordibenzodioxin	47,2
	Summe Heptachlordibenzodioxine (Cl_7-PCDD)	57,2
OCDD:	Octachlordibenzodioxin	56,3
Polychlorierte Dibenzofurane		
TCDF:	2,3,7,8-Tetrachlordibenzofuran	17,0
	Summe Tetrachlordibenzofurane (Cl_4-PCDF)	23300
PeCDF:	Summe 1,2,3,7,8-Pentachlordibenzofuran u. 1,2,3,4,8-Pentachlordibenzofuran	215
	2,3,4,7,8-Pentachlordibenzofuran	38,8
	Summe Pentachlordibenzofurane (Cl_5-PCDF)	924000
HxCDF:	Summe 1,2,3,4,7,8-Hexachlordibenzofuran u. 1,2,3,4,7,9-Hexachlordibenzofuran	13,5
	1,2,3,6,7,8-Hexachlordibenzofuran	11,4
	1,2,3,7,8,9-Hexachlordibenzofuran	9,1
	2,3,4,6,7,8-Hexachlordibenzofuran	248
	Summe Hexachlordibenzofurane (Cl_6-PCDF)	19500
HpCDF:	1,2,3,4,6,7,8-Heptachlordibenzofuran	52,7
	1,2,3,4,7,8,9-Heptachlordibenzofuran	3,8
	Summe Heptachlordibenzofurane (Cl_7-PCDF)	70,8
OCDF:	Octachlordibenzofuran	32,9
Toxizitätsäquivalente nach BGA/UBA:		
	Polychlorierte Dibenzodioxine	123
	Polychlorierte Dibenzofurane	9718
	Summe	9841
Toxizitätsäquivalente (nach I-TEF)		181

JAN

ATTACHMENT B

DIOXIN ANALYTICAL RESULTS

DIOXIN or DIBENZO FURAN ISOMER	ANALYTICAL VALUES(1)					
	DCOP 1(2)	DCOP 2(3)	HEATED COMPOSITE			HEATED HOUSEHLD REFUSE
			400 C(4)	600 C(4)	800 C(4)	800 C(5)
TCDD						
2,3,7,8	34.3	73	136	151	48	54
TOTAL tetra Cl	136	1460	3090	3280	817	1460
PeCDD						
1,2,3,7,8	2.2	40.2	72	63	135	136
TOTAL penta Cl	21.8	282	1700	1860	1610	1630
HxCDD						
1,2,3,4,7,8	3.8	16.4	27	36	23	84
1,2,3,6,7,8	24.3	133	10	28	<10	159
1,2,3,7,8,9	10.3	118	28	10	<10	103
TOTAL hexa Cl	73.1	451	627	835	514	1150
HpCDD						
1,2,3,4,6,7,8	75.4	47.2	294	674	180	364
TOTAL hepta Cl	85	57.2	449	1100	349	437
OCDD	55.1	56.3	944	2630	152	653
TCDF						
2,3,7,8	11.6	17	203	140	25	711
TOTAL tetra Cl	4480	23300	3040	5280	1300	7030
PeCDF						
1,2,3,7,8+1,2,3,4,8	60	215	46	47	12	305
2,3,4,7,8	7.5	38.8	14	<10	<10	468
TOTAL penta Cl	47800	924000	255	246	108	4770
HxCDF						
1,2,3,4,7,8 + 1,2,3,4,7,9	8.3	13.5	13	14	<10	73
1,2,3,6,7,8	5.7	11.4	<10	<10	<10	76
1,2,3,7,8,9	5.2	9.1	<10	<10	<10	52
2,3,4,6,7,8	97.6	248	<10	<10	<10	66
TOTAL hexa Cl	2620	19500	34	132	92	1280
HpCDF						
1,2,3,4,6,7,8	60.2	52.7	<10	60	<10	189
1,2,3,4,7,8,9	5.8	3.8	<10	<10	<10	136
TOTAL hepta Cl	89.4	70.8	<10	99	<10	538
OCDF	80.7	32.9	5780	3060	<10	622
ITEQ	60.4	181	219	221	121	NOT AVAIL (6)

R.S.WARITZ
1/30/92

DIOXMET.WO1
print-to-fit

FOOTNOTES

1) Chlorinated dibenzo-p-dioxin and dibenzofuran analyses. All values are in ng/kg (ppt; 10^{-12}).

2) 2,6,-dichloro-4-(tert.-octyl)phenol (DCOP), made under usual conditions.

3) DCOP heated for 90 minutes at 120-135°C in the presence of 20 percent excess of sulfuryl chloride.

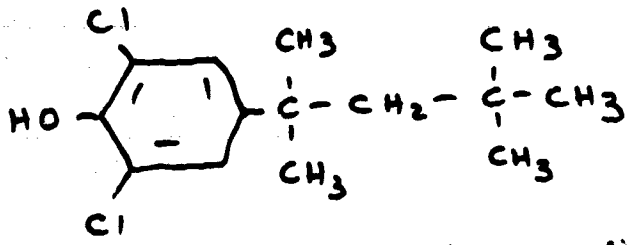
4) Composite containing DCOP. Heated in air at the given temperature. Value given is total of ash and volatiles.

5) European standard household refuse. Conditions the same as in Footnote 3.

6) We have requested this calculation from the contractor, but have not yet received it.

RSW/elm

ATTACHMENT C



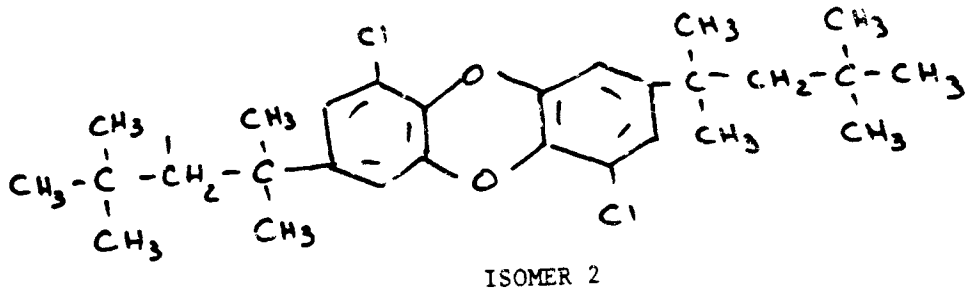
2,6-dichloro-4-(tert.-octyl)phenol (DCOP)

Compound 1

Compound 2

R. S. Waritz
1/28/92

ATTACHMENT D



ISOMER 2

1,6-dichloro-3,8-bis(tert.-octyl)dioxin

R. S. Waritz
January 28, 1992

92 NOV 13 PM 2:01

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