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Comparisons Of Chemical and Biological Data

on Soot Samples From the Binghamton State

Office Building

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Soot samples from two separate samplings of the Binghamton State Office Building (BSOB) have been the objects of a coordinated interdisciplinary study at the New York State Health Department. On May 26, 1981, replicate soot samples were collected from above the ceiling panels of 16 of the 17 floors of the BSOB. Each sample was subjected to exhaustive soxhlet extraction (benzene). One portion of each extract was analyzed for polychlorinated biphenyls (PCBs), another for polychlorinated dibenzofurans (PCDFs) and related compounds. A third portion of all extracts not spiked with PCDDs and PCDFs as part of the chemical analysis procedure was examined using the cell keratinization assay.

Another set of experiments utilized a much larger soot sample collected by a vacuum cleaner on the 3rd and 4th floors of the BSOB shortly after the fire occurred. The bulk of this sample has been used in animal toxicology studies. However, portions of this soot were extracted and analyzed for PCBs, PCDFs, 2,3,7,8-tetrachlorodibenzo-p-dioxin (2,3,7,8-TCDD) and 2,3,7,8-tetrachlorodibenzofuran (2,3,7,8-TCDF). The cell keratinization assay was also applied to an extract of this sample.

The results of each of these studies have been described in detail in separate reports (Smith et al., 1981a, 1981b, 1982; Silkworth et al., 1982; Gierthy et al., 1982). This paper will seek comparisons among the various chemical and biological data sets generated with these samples, and will attempt to determine whether the results are mutually consistent.

Chemical Data

The number of samples which could be analyzed for PCDFs and related trace contaminants is severely limited by the difficulty of the analytical procedure. In contrast, the quantitation of the much more abundant PCBs is a fairly straightforward process; more than 800 PCB analyses have already been reported on BSOB-related samples. If the ratios of PCB to PCDF are approximately constant then the results of the PCB analyses can be used to estimate PCDF levels, with a considerable savings in time and manpower. Table I contains analytical data relevant to the PCB and PCDF (tetra through octa chlorinated) concentrations on soot samples collected from 16 of 17 floors of the BSOB, and on the soot sample used in animal toxicology experiments. The PCB concentrations vary by nearly 3 orders of magnitude, while total PCDF levels vary from not detected (<1.0 ppm) to approximately 1200 ppm. For the 11 samples in which the ratio of total PCDFs to total PCBs has been determined, the total PCDFs measured ranges from 51 ppm to 1200 ppm, and the ratio of PCDF to PCB averages .066 ± .024 (error limits represent one standard deviation). Thus, the total PCDF levels correlate with PCB levels.

More detailed consideration of the data in Table I indicates that the total concentrations of tetra CDFs, penta CDFs and hexa CDFs (groupings which include the isomers predicted (see later) to be most active with respect to acute oral toxicity and keratinization) relative to the total PCDF concentration is relatively constant (Table II). In the 11 samples for which these ratios have been determined, tetra CDFs constitute 33 ± 5%

of the total PCDF mixture, while penta CDFs constitute 40 ± 3%, and the hexa CDFs constitute 18 ± 7% of the total mixture. Thus, the PCB concentration can be used to predict approximate concentrations of each family of chlorinated dibenzofurans in these samples. For illustrative purposes, Table III contains the measured and predicted concentrations.

Further studies will be required to rigorously validate the use of PCB analysis as a surrogate for the more elaborate analytical procedures. Since concentrations of dibenzodioxins and biphenylenes (Stalling, 1981) have not yet been determined in these samples, it cannot be demonstrated that the concentrations of these compounds correlate with PCB concentrations. Further, the samples analyzed to date have all been collected before May, 1981 and have been predominantly obtained from the same location on the 17 floors. The validity of the observed correlation must be tested with more recent samples and with samples taken at other locations; the similarity of the ceiling panel samples and vacuum cleaner sample is encouraging in the latter regard. Finally, the validity of the observed correlation in the very slightly contaminated samples likely to be generated during the final phases of the clean-up should also be tested.

Biological Data

Evaluation of the consistency of the chemical data and the biological data requires knowledge of the concentrations and toxicities of particular congeners believed to be especially active. Because of the very few reference standards available, the laboratories of the Health Department have produced little congener-by-congener analytical data. Therefore, in the following discussions it will be necessary to assume that within a particular isomeric series the relative concentration of a given isomer is comparable to its concentration in a sample earlier subjected to congener by congener analysis (Stalling, 1981; Rappe, 1981).

Among the tetra CDFs, the isomer believed to be most toxic is 2,3,7,8-Tetra CDF (Poland et al., 1977). Stalling and Rappe report that this isomer constitutes 68% and 41% of the tetra CDFs. Based on these results it will be assummed that 2,3,7,8-TCDF constitutes 50% of the total tetra CDF concentration in these samples.

Given the greater toxicity of 2,3,7,8-chlorinated isomers (Poland et al., 1977) the most toxic penta CDF isomers are predicted to be 1,2,3,7,8- and 2,3,4,7,8-penta CDF. Stalling and Rappe report that these congeners comprise together 47% and 53% of the penta CDF mixture. A value of 50% will be assumed in subsequent discussions.

Given the greater toxicity of 2,3,7,8-chlorinated isomers (Poland et al., 1977), the most toxic hexa CDF isomers are predicted to be 1,2,3,4,7,8-, 1,2,3,6,7,8-, 1,2,3,7,8,9- and 2,3,4,6,7,8-hexa CDF. Rappe reports that the total concentration

of three of these isomers in a BSOB sample was 49% of the total
hexa CDF concentration. A value of 50% will be assumed here for
the four isomers.

Knowledge of the relative concentrations of dibenzodioxins
and dibenzofurans will also be required for these discussions.
In the soot sample used in animal toxicology experiments, the
2,3,7,8-TCDD/2,3,7,8-TCDF ratio was determined to be .025 (Smith
et al., 1981b). This ratio will be used in connection with
this sample. However, since analytical data on the dioxin levels
in the remaining samples is not yet available, an estimate of
these concentrations must be made. In a sample analyzed by Rappe
and Stalling, Rappe concluded that the tetra through octa
PCDD/PCDF ratio was about .01, and Stalling concluded that it was
less than .02. In a heavily contaminated soot sample, Smith et
al (1981a) concluded that the 2,3,7,8-TCDD/2,3,7,8-TCDF ratio
averaged .015. The average ratio observed in the three samples
was .017; this value will be assumed for the ceiling panel
derived soot samples.

Based on Stalling's report (1981), the biphenylene/dibenzo-
furan ratio in a sample was less than .067. This value will of
necessity be used in subsequent discussions. Efforts are
presently underway to obtain experimental data on the soot
samples currently under discussion to place these estimates on a
firmer basis.

a. Animal Toxicology Experiments

It is difficult to rigorously demonstrate consistency
between results obtained via chemical analysis and acute toxicity
data for a number of reasons. The chemical data is incomplete;

not all classes of toxicants have been quantified,and the concentrations of individual congeners have not been established. More important, however, very limited data is available on the acute oral toxicities of individual PCDFs, PCDDs or Polychlorinated Biphenylenes. Nevertheless, despite these and other difficulties, crude comparison of this data will be attempted.

A useful first step is to express the observed acute oral toxicity of the soot in terms of "2,3,7,8-TCDD equivalents", i.e., the concentrations of 2,3,7,8-TCDD, that, in an inert matrix, would produce the observed LD_{50}. An extract of soot when administered to guinea pigs in aqueous suspension exhibited an LD_{50} equivalent to 327 mg soot/kg. When 2,3,7,8-TCDD was administered under identical conditions, it exhibited an LD_{50} of 19 ug/kg. If the soot in fact had contained only 2,3,7,8-TCDD at 58 ug/g, its extract would be predicted to exhibit an LD_{50} of 327 mg soot equivalents/kg. Therefore, the "2,3,7,8-TCDD equivalent" contamination of the soot is 58 ug/g.

The chemical data can then be used to "predict" the "2,3,7,8-TCDD equivalent" concentration of the soot, based on known toxicities of the components. This is a complicated task, since no data is available on the LD_{50}s of dibenzofurans in guinea pigs other than 2,3,7,8-tetra CDF, and since very limited data is available on the PCDDs. The following assumptions will therefore be made about the LD_{50}s of these compounds: (1) The ratio of the LD_{50}s of a particular PCDF congener and 2,3,7,8-tetra CDF will be the same as the ratio of the LD_{50}s of the correspondingly substituted PCDD congener and 2,3,7,8-TCDD.

There is no direct experimental data to support this assumption. (2) The LD_{50}s of PCDFs and PCDDs lacking chlorines on all four lateral positions will be sufficiently high that their influence can be ignored in this calculation. This assumption is based on the LD_{50}s in guinea pigs of 2,8-diCDD, 2,3,7-triCDD, and 1,2,4,7,8-penta-CDD. All have LD_{50}s more than 450 times higher than that of 2,3,7,8-Tetra CDD itself (Table IV). (3) Introduction of a single additional chlorine substituent on a 2,3,7,8-substituted congener has essentially no effect on the congener's guinea pig LD_{50}. This assumption is based on comparison of the LD_{50}s of 2,3,7,8-TCDD and 1,2,3,7,8-tetra-CDD (Table IV). (4) Introduction of two additional chlorine substituents on a 2,3,7,8-chlorinated congener raises its LD_{50} by a factor of at least 29. The assumption is based on comparison of the LD_{50}s of 1,2,3,4,7,8-, 1,2,3,6,7,8-, and 1,2,3,7,8,9-hexa CDD and 2,3,7,8-tetra CDD (Table IV). (5) The LD_{50}s of compounds with more than 6 chlorines will be sufficiently large that their influence can be ignored in this calculation. This assumption is based on comparison of the LD_{50}s of 1,2,3,4,6,7,8-hepta CDD and 2,3,7,8-tetra CDD (Table IV).

These assumptions require that attention be focussed only on the tetra, penta, and hexasubstituted PCDDs and PCDFs. The concentration of 2,3,7,8-TCDF in the sample used in animal toxicology experiments was measured at 48 ppm; since the data in Table IV indicates that the LD_{50} of 2,3,7,8-tetraCDF is about three times that of 2,3,7,8-TCDD, this is equivalent in terms of acute toxicity to a 2,3,7,8-TCDD concentration of ca. 16 ug/g.

Based on assumption (2), other tetra CDFs can be neglected in this calculation. The penta CDFs were measured at 120 ug/g. If 1,2,3,7,8- and 2,3,4,7,8-penta CDF together constitute 50% of the penta CDFs, and if their LD_{50}s are equal to that of 2,3,7,8-TCDF, this is equivalent in terms of acute toxicity to a 2,3,7,8-TCDD concentration of ca. 20 ug/g. Based on assumption (2), other penta CDFs can be neglected in this calculation. The hexa CDFs have been measured at 70 ug/g. The isomers believed to have the lowest LD_{50}s (1,2,3,4,7,8-, 1,2,3,6,7,8-, and 2,3,4,6,7,8-hexa CDF) are expected to comprise 50% of the total hexa CDF mixture. Since, based on assumption (4), their LD_{50}s are 29 times higher than that of 2,3,7,8-TCDF, this is equivalent to a 2,3,7,8-TCDD concentration of 0.4 ug/g. Thus, the PCDFs are calculated to constitute a "2,3,7,8-TCDD equivalent" concentration of 36 ug/g.

The concentration of 2,3,7,8-TCDD itself has been measured at 1.2 ppm in this sample. Other tetrachlorinated dibenzodioxins are predicted to have much higher LD_{50}s and can be ignored. The concentration of other PCDDs in this sample are unknown, but are likely to be comparable to the TCDDs. Thus, the dioxins as a whole probably have a negligible influence on the soot's "2,3,7,8-TCDD equivalent" concentration.

Stalling (1981) has reported on the presence of polychlorinated biphenylenes in a soot sample from BSOB; he cites unpublished results by Dr. Alan Poland that suggests that the toxicity of the 2,3,6,7 congener is comparable to that of 2,3,7,8-tetra CDD. If Stalling's ratio of biphenylene to dibenzofuran is (.067) is assummed to hold for all of these

compounds, and if it is assummed that the biphenylenes have acute oral toxicities three times that of the corresponding dibenzofurans, it can be calculated that the biphenylenes will contribute about 0.2 times as much "2,3,7,8-TCDD equivalent" activity as the dibenzofurans. Thus, to a very crude approximation, the polychlorinated biphenylenes account for a "2,3,7,8-TCDD equivalent" concentration of 7 ppm.

In summary, the dibenzofurans and the tetra CDDs are estimated to constitute a "2,3,7,8-TCDD equivalent" activity of 37 ug/g. Together, the remaining dibenzodioxins and the biphenylenes probably provide a significant but smaller "2,3,7,8-TCDD equivalent" activity. This calculation is in good, probably somewhat fortuitous agreement with the observed activity in the soot-equivalent to a 2,3,7,8-TCDD concentration of 58 ug/g.

Since considerable effort has been devoted to animal toxicology experiments on a single large sample of soot, it is important to assess whether this sample is reasonably typical. The data in Table I indicates that the average PCB concentration in 16 samples collected above the ceiling panels at the BSOB is 7200; the PCB concentration in this sample is 5,000 ppm. The average total PCDF concentration on 14 such samples was ppm; the total PCDF concentration in this sample is 320 ppm. The average ratio of total PCDF to PCB in the 12 samples for which this is well defined is .066; the ratio for this sample was .063. The proportions of tetra- penta-, and hexa CDFs in this sample are similar to those in the ceiling panel samples (Table II). Thus, the sample used in animal toxicology experiments appears

comparable to the samples collected from above the ceiling panels, based on presently available data.

b. Cell Keratinization Assay

Development of the cell keratinization assay based on an in vitro keratinization model (Knutson et al., 1981) has been pursued because of its potential use as an alternative or supplement to chemical analysis. Both applications demand that the biological and chemical methods generate mutually consistent results. One question can be answered fairly readily. Do the two methodologies agree which samples fall into particular broad categories of contamination? The samples and blanks run as part of this program exhibit four broad categories of contamination. Blanks did not exhibit positive responses in this assay. A single sample (floor 1) exhibited activity equivalent to 0.01 - 0.10 ppm 2,3,7,8-TCDD; chemical analysis detected only 0.2 ppm Tetra-CDF. Three samples (floors 4,6, and 14) exhibited activities near 0.10 - 1.0 ppm; chemical analysis confirmed low levels of PCDFs in these samples (total PCDFs of 51, 76, and 87 ppm). The remaining samples in which PCDFs were detected chemically exhibited activities ranging from 1.1 - 11 ppm to 5.3 - 53 ppm. Chemical analysis confirmed that these samples were more heavily contaminated (total PCDFs of 410 , 200, 320, 1200, 400, 750, and 670 ppm). These results are collected together in Table V. They suggest that the keratinization assay results correlate with chemical data.

It is markedly more difficult to determine whether the activity observed in the cell keratinization assay is quantitatively consistent with chemical analysis. Little

published information exists to relate the keratiniation activities of the various compounds present in the soot to one another. However, the following assumptions will be made to permit a crude calculation: (1) The ratios of the activity of a particular dibenzofuran congener to 2,3,7,8-TCDF is equal to that of the ratio of the activity of the corresponding dibenzodioxin congener to 2,3,7,8-TCDD. There is no direct support for this assumption. (2) 2,3,7,8-Tetra CDF is 1/20 as active as 2,3,7,8-TCDD (Knutson et al., 1980). (3) Congeners not substituted at all four lateral positions are sufficiently inactive to be neglected. This assumption is based on comparison of the activities of 2,3-, 2,7-, 1,6-, 1,3,6,8-, 1,3,7,8-, and 2,3,7- chlorodibenzodioxins to 2,3,7,8-tetra CDD. (Knutson et al., 1980) (Table VI). (4) Introduction of a single additional chlorine on a 2,3,7,8 chlorinated nucleus decreases activity by a factor of 2. This assumption is based on a comparison of the activities of 1,2,3,7,8-Penta CDD and 2,3,7,8-tetra CDD (Knutson et al., 1980) (Table VI). (5) Introduction of two or more chlorines depresses activity sufficiently to make the activity of such compounds negligible. This assumption is based on comparison of the activities of 1,2,3,7,8,9-hexa CDD and 2,3,7,8-tetra CDD (Knutson et al., 1980) (Table VI). (6) Polychlorinated biphenylenes are 1/2 as active as the corresponding dibenzodioxin. This generalization is based on comparison of the activities of 2,3,6,7-tetra CB and 2,3,7,8-tetra CDD (Knutson et al., 1980) (Table VI).

As a direct result of assumptions (3) and (5), the bulk of keratinization activity will reside in tetra- and penta-

chlorinated compounds. As already discussed, 2,3,7,8-tetra CDF is predicted to be by far the most active tetra CDF, and expected to constitute 50% of the tetra CDF mixture. Since 2,3,7,8-tetra CDF is 1/20 as active as 2,3,7,8-TCDD, the "2,3,7,8-TCDD equivalent" activity due to this compound can be obtained by dividing the total tetra CDF concentration by 40. Similarly, the "TCDD equivalent" activity of the two most active penta CDFs can be estimated by dividing the total penta CDF concentration by 80. The calculated "2,3,7,8-TCDD equivalent" activity due to PCDFs is compared to the experimentally observed value for a number of samples in Table VII.

The PCDDs will make a significant contribution to the cell keratinizing activity of these samples; although they are estimated to be 1/50 to 1/100 as abundant as the PCDFs, they may be 20 times as potent in the assay. The polychlorinated biphenylenes may be even more important factors in this analysis. Stalling's data suggests that they may be 1/10 to 1/20 as abundant as the PCDFs. However, they are reported to be 10 times as active. Thus, the calculated values in Table VII are likely to be below the values that would be calculated if more complete analytical data were available. However, in view of the large uncertainties present in these calculations and the data upon which they are based, the calculated and experimental data are in fair agreement.

It should be noted that the soot sample used in the animal toxicology experiments exhibited a cell keratinizing activity of 2-20 ppm "2,3,7,8-TCDD Equivalents", and a calculated activity of 4 ppm due to PCDFs. This differs from the "2,3,7,8-TCDD

equivalents" calculated and observed in the animal toxicology experiments This does not represent a discrepancy in the data. Rather, it is due primarily to the large difference between the ratios of the guinea pig LD_{50}s for 2,3,7,8-TCDF and 2,3,7,8-TCDD, and the corresponding ratios of cell keratinization activity.

Conclusions

(1) Available chemical data indicate that the relative concentrations of PCBs, tetra-, penta-, and hexa-CDFs, and total PCDF are similar in soot samples taken from above the ceiling panels of the BSOB, and in a sample collected by vacuum cleaner during the early stages of the clean-up. If this relationshiip is valid for samples collected at other times and from other locations, the PCB analysis can serve as a useful surrogate for the more difficult analytical procedures. (2) A soot sample exhibited an LD_{50} in guinea pigs equivalent to 58 ppm 2,3,7,8-Tetra CDD. If certain assumptions are made about the chemical composition of this sample and the LD_{50}s of the compounds therein, it can be calculated that the PCDFs, tetra CDDs, and the biphenylenes should account for ca. 45 ppm "2,3,7,8-TCDD equivalent" activity. Since this calculation ignores other chlorinated dioxins, it is in good (probably fortuitous) agreement with the observed value. Based on these results, there appears to be no basis for proposing unusual synergistic or antagonistic effects among the components in this mixture. (3) The cell keratinization assay can reliably distinguish among samples containing widely differing concentrations of PCDFs. If certain assumptions are made about

the chemical composition of compounds therein, it can be calculated that the observed keratinizing activity in these extracts is generally plausible. (4) Chemical analysis and the cell keratinization assay suggest that the soot used in animal toxicology studies is fairly typical of the soot samples collected from above the ceiling pannels of the BSOB.

TABLE I

Concentrations (ppm) of Polychlorinated Biphenyls and Polychlorinated Dibenzofurans in Soot Samples Taken From the Binghamton State Office Building

Floor #	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	Ave	3-4[f]
PCBs[a]	28		1300	840		2800	6600	1800	23000	9600	21000	11000	3400	930	10000	9200	6500	7200	5000
PCDFs[b]																			
Tetra CDF	0.2		<8[g]	16	220	23	190	70	320	140	250	d	d	32	300	h	220	145	100
Penta CDF	<0.2[g]		<9[g]	21	280	36	180	79	440	170	360	d	d	31	310	150[h]	260	165	120
Hexa CDF	<0.3[g]		<11[g]	13	180	14	35	32	290	84	260	d	d	e	56	89[h]	140	86	70
Hepta CDF	<0.3[g]		<12[g]	1.2	62	3	3.7	14	100	6.5	97	d	d	5.8	71	33[h]	32	31	20
Octa CDF	<0.3[g]		<14[g]	<1.2	21	0.5	--	3	35	2	31	d	d	2.8	17	11[h]	15	11	4
Total PCDF	--		--	51	760	.76	410	200	1200	400	1000	--	--	87	750		670	438	310
Ratio Total PCDF conc. / PCB conc.				.061		.027	.062	.11	.052	.042	.048			.094	.075		.103	.066	.062

(a) quantitated as Arochlor 1254; data uncorrected for recovery

(b) correction for recovery incorporated

(c) not sampled because of dissimilar ceiling construction

(d) data not used because of poor recovery of internal ^{37}Cl-Tetra CDF standard (<10%)

(e) data lost because of instrumental malfunction; for purposes of calculation of total PCDF, it is assumed that hexa CDF is ½ the concentration of penta (cf. Table 2)

(f) soot collected by vacuum cleaner and used in animal toxicology studies

(g) detection limits are per congener, not per chlorination number

(h) data not corrected for recovery. Instrument malfunction caused loss of data on ^{37}Cl-Tetra CDF recovery

Table II

Relative Proportions of Tetra-, Penta-, Hexa-, Hepta- and Octachlorodibenzofurans in Soot Samples Taken from the Binghamton State Office Building[a]

Floor #	4	5	6	7	8	9	10	11	14	15	17	Ave[b]	3-4[c]
Tetra CDF	31	29	30	46	35	27	35	25	37	39	33	33 ± 5	32
Penta CDF	41	37	47	44	40	37	41	36	36	41	39	40 ± 3	38
Hexa CDF	25	24	18	9	16	24	21	26	--	7	21	18 ± 7	22
Hepta CDF	2	8	4	1	7	8	2	10	7	10	5	6 ± 3	6
Octa CDF	<1	3	1	<1	1	3	<1	3	3	2	2	---	1

(a) Expressed as percent of total PCDF in sample.

(b) Error limits represent one standard deviation.

(c) Soot sample used in animal toxicology studies.

Table III

Comparison of Predicted[a] (and Observed) Concentrations (ppm) of PCDFs in BSOB Soot Samples

Floor #	1	3	4	6	7	8	9	10	11	14	15	17	3-4
Tetra CDF	0.6(0.2)	26(8)	17(16)	56(23)	133(190)	39(70)	460(320)	190(140)	420(250)	19(32)	200(300)	130(220)	100(100)
Penta CDF	0.9(<.2)	30(<9)	19(21)	64(36)	151(180)	45(79)	530(440)	220(170)	480(360)	21(31)	230(310)	150(260)	115(120)
Hexa CDF	0.3(<.3)	16(<11)	10(13)	33(14)	79(35)	23(32)	270(290)	115(84)	250(260)	11(--)	120(56)	78(140)	60(70)
Hepta CDF	0.1(<.3)	5.6(<12)	3.6(1.2)	12(3)	28(3.7)	8.4(14)	99(100)	41(6.5)	90(97)	5(5.8)	43(71)	28(32)	22(20)
Octa CDF	.04(<.3)	2(<13)	1.3(<1.2)	4.2(0.5)	10(--)	3(3)	35(35)	15(2)	32(31)	1.4(2.8)	15(17)	10(15)	8(4)
Total PCDF	1.9	80	51(51)	160(76)	400(410)	120(200)	1400(1200)	580(400)	1300(1000)	57(87)	610(754)	400(670)	300(310)

(a) Prediction based on PCB levels and average ratio calculated in Table I and II

Table IV

Influence of Structure and Chlorination Pattern on Guinea Pig
Oral LD_{50}s (Male, Hartley, 200-250g)

Compound	LD_{50}(ug/kg)
2,3,7,8-Tetra CDD	2.5[a]
2,3,7,8-Penta CDF	5-10[b]
1,2,3,7,8-Penta CDD	3.1[c]
1,2,3,4,7,8-Hexa CDD	73[c]
1,2,3,7,8,9-Hexa CDD	60-100[c]
1,2,3,6,7,8-Hexa CDD	70-100[c]
1,2,3,4,6,7,8-Hepta CDD	>600[c]
1,2,4,7,8-Penta CDD	1,125[c]
2,3,7-Tri CDD	29,444[c]
2,8-Di CDD	730,000[c]

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Pharmacol. 44, 335-356.
0

Table V

Comparison of the Observed Keratinization Activities with Total PCDF Concentrations

Floor #	Observed "2,3,7,8-TCDD Equivalents(ppm)	Total PCDF Concentrations (ppm)
1	.01-1	__ b
6	0.1-1.0	76
4	.11-1.1	51
14	.12-1.2	87
3	1.2-12	__ b
9	1.1-11	1200
8	1.6-16	200
3-4[a]	2-20	310
10	3.2-32	400
15	4.0-40	750
17	4.0-40	670
7	5.3-53	410

[a]Soot used in animal toxicology experiments

[b]Total concentration not defined. (cf. Table I)

Table VI

Influence of Structure and Chlorination Pattern on Relative
Activity in the Cell Keratinization Assay[a].

Compound	Relative Activity
2,3,7,8-Tetra CDD	1
2,3,7,8-Tetra CDF	0.05
2,3,6,7-Tetrachlorobiphenylene	0.5
1,2,3,7,8-Penta CDD	0.5
2,3,7-Tri CDD	0.01
1,3,7,8-Tetra CDD	0.01
1,2,3,7,8,9-Hexa CDD	0.005
1,3,6,8-Tetra CDD	< .003
1,6,-DiCDD	< .001
2.7-DiCDD	< .001
2.3-DiCDD	< .001

(a)   Data adapted from J.C. Knutson and A. Poland (1980).
Keratinization of mouse teratoma cell line XB produced by
2,3,7,8-tetrachlorodibenzo-p-dioxin: an in vitro model of
toxicity, Cell 22, 27-36.

Table VII

Comparison of the Observed Keratinization Activity in BSOB Soot Samples with Value Predicted based on PCDF Concentrations

Floor #	Observed "2,3,7,8-TCDD equivalents" (ppm)	Calculated "2,3,7,8-TCDD equivalents" (ppm) PCDFs only
1	.01-.1	(b)
6	0.1-1.0	1
4	.11-1.1	1
14	.12-1.2	1
3	1.2-12	(b)
9	1.1-11	10
8	1.6-16	3
3-4[a]	2-20	4
10	3.2-32	6
15	4.0-40	10
17	4.0-40	9
7	5.3-53	7

(a) Sample used for animal toxicology studies.

(b) PCDFs not detected in chemical analysis.

Smith, R.M., O'Keefe, P.W., Hilker, D.L., Jelus-Tyror, B.L., and Aldous, K. (1981a). Analysis of 2,3,7,8-tetrachlorodibenzofuran and 2,3,7,8-tetrachlorodibenzo-p-dioxin in a soot sample from a transformer explosion in Binghamton, New York. New York State Department of Health Report, February 20, 1981.

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