file Aroclor Quality

WGK ANALYTICAL RESEARCH AND DEVELOPMENT REPORT No. 2724 June 30, 1975

OTHER LOCATIONS	GENERAL OFFICE	W. G. KRUMMRICH PLANT
	R. Munch - T1B R. Keller - T1B	W. L. Smull W. C. Engman C. F. Buckley E. E. Stewart ~~A. D. Leisy~~ File

TITLE:

Analytical Research and Development - Progress Report

PERSONNEL:

H. L. Campbell (H. J. Horner)

PROBLEM:

Isomeric composition of Aroclors 1242 and 1254.

JUSTIFICATION:

Provide gas chromatographic, PCB methods with more informational content.

SUMMARY:

To date, twelve chlorobiphenyl isomers have been found to fit reasonably well into chromatographic elution patterns of Aroclor 1242.

A comparison of 1242 composition by methods is presented, and a synthetic isomeric standard (1242) has been constructed.

Work to determine the principal isomeric composition of Aroclor 1254 is underway.

H. L. Campbell

dy

CONFIDENTIAL

This report is the property of Monsanto Company and the recipient is responsible for its safekeeping and disposition. It contains confidential information of Monsanto Company which must not be reproduced, revealed to unauthorized persons or sent outside the company without proper authorization. This report is to be retained in a secure file or destroyed.

WGK 899

Details

The Krummrich Plant AR-D Group performs PCB residue analyses on all non-routine biological samples and some special plant environmental investigations. Two different, electron capture gas chromatographic (EC/GC) methods - both interfaced with a data processing system - are used to make the determinations. While background and experience has helped to identify the molecular composition of some of the observed peaks (i.e. number of chlorines per molecule), little information is available as to their actual isomeric composition.

The present work is an attempt to relate chromatographic characteristics of individual chlorobiphenyl isomers with the observed peaks of our analytical chromatograms. The structural information obtained, can eventually be used to establish amplification and/or degradation of Aroclor components in ecological systems; and hopefully, provide a means of improving quantitation on the basis of actual component concentrations. To date, twelve chlorobiphenyls have been found to fit reasonably well into the elution patterns of Aroclor 1242 by both GC methods (Figs. 1 and 2).

Table I gives the weight percent of the EC/GC peak in 1242 as represented by the given isomer(s). A comparison is made between our methods and GC-mass spec data from a literature reference (1). The latter does not give isomeric structure, but reports composition by number of chlorines. As expected, the largest differences are shown for overlapping and incompletely resolved peaks. The total amount of 1242 accounted for by method PCB-55 falls the nearest to that of the GC-mass spec analysis. This is due to the better resolution provided by the method's parameters.

From the data obtained, a synthetic 1242 isomeric standard has been constructed (Fig. 3), representing a nominal 66% by weight of this Aroclor. The standard is now being evaluated as a means of quantitizing 1242 residues in samples from the actual isomeric concentrations.

Similar work is underway with a number of penta and hexachlorobiphenyls. From their EC/GC characteristics we hope to establish Aroclor 1254's principal isomeric composition, and eventually construct a suitable synthetic mixture.

Reference

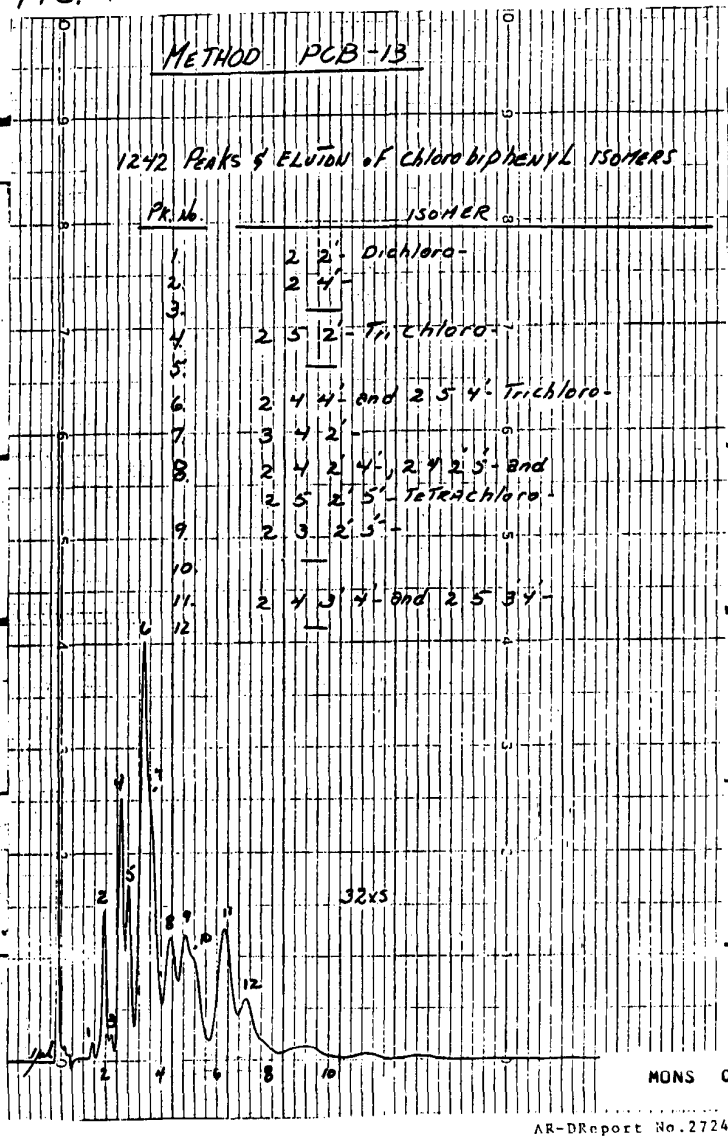
1. J. Chromatog. Sci., 11, 366 (1973).

MONS 048799

H. L. Campbell

dy

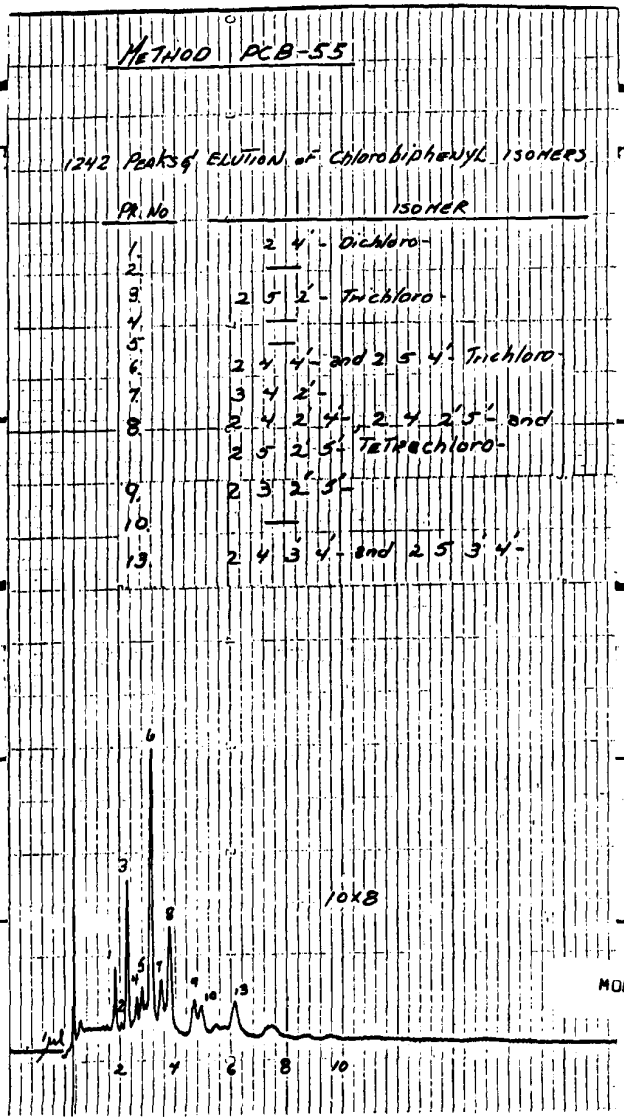
FIG. 1



MONS 048800

AR-DReport No. 2724
7/1/75

FIG. 2



MONS 048801

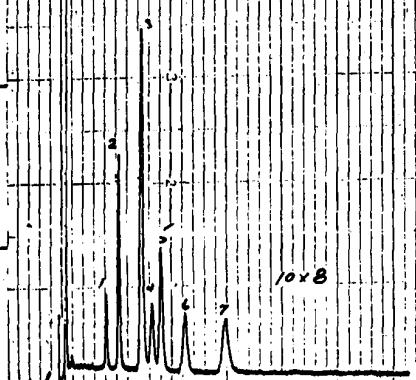
AR-D Report
2724
7/1/75

FIG. 3

METHOD PCB-55

AROCLOR 1242 ISOMERIC STANDARD

PK. No.	ISOMER	Electron Capture Response (relative To 2 4' Dichloro-)
1	2 4'- Dichloro-	1.00
2	2 5 2'- Trichloro-	1.25
3	2 5 4'-	2.39
4	3 4 2'-	1.55
5	2 5 2' 5'- Tetrachloro-	2.76
6	2 3 2' 5'-	1.82
7	2 5 3' 4'-	2.21



MONS 048802

AR-II Report
2724
7/1/75

BLE I A COMPARISON OF AROCLOR 1242 COMPOSITION BY METHODS

ISOMER	Method PCB-13	Method PCB-55	LITERATURE REFERENCE (1) Peak No. (2)	No. of Chlorines	wt %
2 2'- Dichloro-	4.2	-	16	2	2.9
2 4'-	7.6	9.5	21	2	11.3
2 5 2'- Trichloro-	15.0	16.0	28	3	8.2
2 4 4' and 2 5 4'-	23.8 - 29.7 (3)	12.2 - 17.7	37	3	11.5
3 4 2'-	33.7 (3)	5.4	40	3	11.1
2 4 2' 4', 2 4 2' 5' and 2 5 2' 5'- Tetrachloro-	7.0 - 12.0	9.8 - 16.8	41	4	8.8
2 3 2' 5'-	12.2 (3)	3.0	54	4	4.5
2 5 3' 4' and 2 4 3' 4'-	7.8 - 8.3	4.2 - 5.4	70	4	9.3
% TOTALS:	78-89	60-74			67.6

MONS 048803

NOTES:

(1) WEBB, R.G., MCCALL, A.C., J. CHROMATOG. SCI. 11, 366 (1973) - FROM GC/MS DATA

(2) RETENTION TIME RELATIVE TO p p'- DDE = 100

(3) AREAS of PEAK and shoulder summed and reported as one.

AR-D Report 2724
7.1.75