UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
WASHINGTON, D.C. 20460

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EPA United States Environmental Protection Agency **Office of Pesticide Programs**

MEMORANDUM

SUBJECT: **Data Evaluation Report for Estimating the Soil Adsorption Coefficient of PXTS**

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DP Barcode (s): ~~D204272~~ D299908

Pesticide Chemical No.: 006929

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Attached please find the Data Evaluation Report (DER) for estimating the soil adsorption coefficient of PXTS (Polyxylenoltetrasulfide) submitted by the Akzo Nobel Functional Chemical LLC.

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EXECUTIVE SUMMARY:

The K_{oc} values for PXTS were estimated using an HPLC estimation method. The experiment was conducted in accordance with OECD Method 121 "Estimation of the Adsorption Coefficient (K_{oc}) on Soil and Sewage Sludge Using High Performance Liquid Chromatography (HPLC)", and in compliance with the GLP standards (Title 40 CFR, Part 160) and OECD Standard ENV/MC/CHEM(98)17. The log K_{oc} value for PXTS was determined using an HPLC estimation method by comparing the chromatographic retention time of the test compound with a series of reference compounds. The HPLC system used was the Hewlett-Packard Model 1090 with a ZORBAX CN column and variable wavelength UV detection. The logarithms of the capacity factors were plotted against published log K_{oc} values to establish a linear regression calibration. The capacity factors of PXTS were used in conjunction with the linear regression equation to calculate the log K_{oc} range for PXTS.

The peak retention times for PXTS ranged from 1.374 ± 0.0906 minutes to 5.231 ± 0.007 minutes. The capacity factors (k') for the minimum and maximum retained PXTS components were then calculated based on the above retention time range. The corresponding adsorption coefficients (Log K_{oc}) for PXTS ranged from <0 to 4.76 ± 0.0058. PXTS eluted as a broad band of mostly unresolved peaks.

Results Synopsis:

Product/Chemical: PXTS
Estimated log K_{oc} (HPLC): <0 to 4.76 ± 0.0058

This study was not conducted according to the EPA guideline requirements for an adsorption/desorption study in soil. As an actual soil study was not conducted, it is unknown whether this is an acceptable replacement for the determination of the K_{oc} values for PXTS. Consequently, this study is considered unacceptable to support registration of this chemical.

I. MATERIALS AND METHODS

GUIDELINE FOLLOWED: The soil adsorption coefficient (K_{oc}) for PXTS was estimated using OECD Method 121 "Estimation of the Adsorption Coefficient (K_{oc}) on Soil and Sewage Sludge Using High Performance Liquid Chromatography (HPLC)."

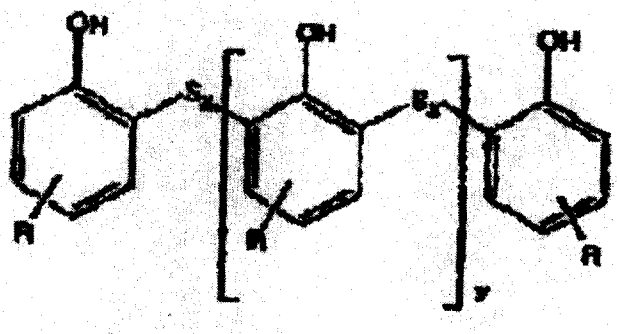
COMPLIANCE: All phases of this study were conducted in compliance with GLP standards (Title 40 CFR, Part 160) and OECD Standard ENV/MC/CHEM(98)17

A. MATERIALS:

1) Test Material PXTS

Chemical Structure:

Description: PXTS is a dark solid supplied by Akzo Nobel (Batch #1685-23, Bottle #2).



Purity: 100% (Expiration date March 28, 2005)

Storage conditions of test chemicals:

The test substance was received from Akzo Nobel on April 1, 2002. It was assigned Wildlife International Ltd. identification number 5942 upon receipt and was stored under ambient conditions.

Physico-chemical properties of PXTS:

Parameter	Values
Water solubility	NR
Vapour pressure	NR
UV absorption	NR
pK_a	NR
K_{ow}	NR
Stability of Compound at room temperature	NR

* A certificate of analysis was provided in Appendix 2 of the Study Report.

2. Soil Characteristics

Soils were not used in this study. The adsorption constant was determined by the HPLC estimation method (OECD 121).

C. STUDY DESIGN:

1. Preliminary study:

A preliminary study was not conducted.

2. Definitive study experimental and analytical conditions:

Retention times of the test substance and reference standards were determined using a HPLC equipped with a variable wavelength UV detector. Seven reference standards were injected individually prior to and after the test substance to determine retention times. The concentrations of the reference standards were adjusted as necessary to give a detector response of at least 600 milli-absorbance units for peak height. The reference standards used were the following: thiourea, phenol, aniline, naphthalene, phenanthrene, endosulfan, and 1,1-bis(p-chlorophenyl)-2,2,2-trichloroethane (DDT). The test substance was injected in triplicate after the initial reference standard injections and was analyzed under the same chromatographic conditions. Each of the injections of the test solution gave a detector response of at least 500 milli-absorbance units for the peak height of the most sensitive PXTS peak.

Sample analysis was conducted using the Hewlett-Packard Model 1090 HPLC system with variable wavelength UV detection under the following conditions:

Column:	ZORBAX CN; 4.6 x 150 mm; 5 µm particle size
Detector:	Hewlett-Packard Model 1100 Variable Wavelength UV Detector
Mobile Phase:	Acetonitrile:NANOpure® water; 55:45, v:v
Flow Rate:	1.0 mL/minute
Stop Time:	10.0 minutes
Oven Temperature:	40°C
Injection Volume:	150 µL
Wavelength:	200 n

Capacity factors were calculated for the reference standards and PXTS using thiourea to estimate the dead time. The logarithms of the capacity factors were then plotted against published log K_{oc} values to establish a linear regression calibration. The capacity factors of PXTS were used in conjunction with the linear regression equation to calculate the log K_{oc} range

for PXTS.

3. Description of analytical procedures:

The analytical procedures and methodology were one in the same for this study as the experimental procedure included running the samples on a HPLC system.

II. RESULTS AND DISCUSSION

A. TEST CONDITIONS:

Details on the HPLC operating conditions are reported previously in section C.2. Additional information on the conditions of the test system were not provided.

B. MASS BALANCE:

Mass balance was not evaluated as a part of this study.

Table 1: Estimated Log K_{oc} Values for PXTS and Reference Standards Determined by HPLC

Sample	Injection Volume (µL)	Retention Time (minutes)	Capacity Factor (k')[a]	Log k'[b]	Log K_{oc}[c]
1A (beginning)	100	1.479	-0.217	NA	<0 (-0.8)[d]
1B (beginning)		1.322	-0.3	NA	<0 (-0.8)[d]
1C (beginning)		1.322	-0.3	NA	<0 (-0.8)[d]
Mean Values					<0 (-0.8)[d]
1A (end)	100	5.236	1.772	0.2484	4.77
1B (end)		5.234	1.771	0.2482	4.76
1C (end)		5.223	1.765	0.2467	4.76
Mean Values					4.76
Phenol	100	2.417	0.28	-0.5536	1.32[e]
		2.437	0.29	-0.5375	
Aniline	25	2.466	0.305	-0.5151	2.07[e]
		2.469	0.307	-0.5128	
Naphthalene	25	3.464	0.834	-0.079	2.75[e]
		3.466	0.835	-0.0784	
Phenanthrene	50	4.158	1.201	0.0796	4.09[e]
		4.152	1.198	0.0785	
Alpha-Endosulfan	100	4.724	1.501	0.1763	4.09[e]
		4.711	1.494	0.1743	
DDT	50	6.47	2.425	0.3847	5.63[e]
		6.415	2.396	0.3795	

[a] Capacity factor (k') is the standard retention time minus the mean column dead time (1.889 minutes for thiourea) divided by the mean column dead time.
[b] Values obtained using Excel 2000 in full precision mode.
[c] Log K_{oc} values are based on literature values (OECD 2001).
[d] Values in parenthesis are extrapolated values.

C. ADSORPTION:

The peak retention times for PXTS ranged from 1.374 ± 0.0906 minutes to 5.231 ± 0.007 minutes. The capacity factors (k') for the minimum and maximum retained PXTS components were then calculated based on the above retention time range. The corresponding adsorption

coefficients (Log K_{oc}) for PXTS ranged from <0 to 4.76 ± 0.0058. PXTS eluted as a broad band of mostly unresolved peaks.

D. DESORPTION:

Desorption was not included as a part of this study.

III. STUDY DEFICIENCIES:

No deficiencies were noted in the study. The study could not be reviewed against any of the EPA guidelines for adsorption/desorption as this was not a soil study, but rather an analytical study following OECD methodologies.

This absorption coefficient estimation method may not be the most accurate evaluation of this particular chemical due to the lack of defined peaks from the test substance as it was run through the HPLC system.

IV. STUDY ACCEPTABILITY

This study was performed according to OECD guideline 121, Estimation of Adsorption Coefficient (K_{oc}) in Soil and Sewage Sludge Using High Performance Liquid Chromatography (HPLC). This procedure is not a recommended procedure of OPP; Therefore, it is considered a screening study and is unacceptable for use in supporting registration of this chemical.

V. REFERENCES:

1. Organisation for Economic Cooperation and Development. 2001. OECD Guideline for the Testing of Chemicals, Proposal for a New Guideline 121: Estimation of the Adsorption Coefficient (K_{oc}) on Soil and on Sewage Sludge Using High Performance Liquid Chromatography (HPLC).

2. American Society for Testing and Materials. 1991. Standard Specification for Reagent Water. D1193-91, ASTM Section II Water and Environmental Technology, Vol. 11.01: 45-47.

File: C:/Myfiles/2004 Reports/PXTS/ Data Evaluation Report for Estimating the soil Adsorption Coefficient of PXTS . Wpd

CC: Siroos Mostaghimi/RASSB
Chemical Files