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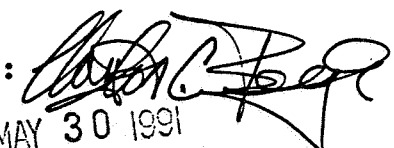
DATA EVALUATION RECORD

STUDY IDENTIFICATION:

Wong, A.S., and Crosby, D.G. 1981. Photodecomposition of pentachlorophenol in water. J. Agric. Food Chem. 29:125-130.

REVIEWED BY:

Clayton C. Beegle, Entomologist
Review Section 1, EFGWB

Signature: 

Date: MAY 30 1991

APPROVED BY:

Paul J. Mastradone, Chief
Review Section 1, EFGWB

Signature: 

Date: MAY 30 1991

TYPE OF STUDY: Photolysis in water (161-2).

MAY 30 1991

CONCLUSIONS:

EFGWB concludes that this study does not satisfy the data requirements for an aqueous photolysis study and will be considered as supplemental. It is unlikely that the following deficiencies can be corrected so as to make the study acceptable. EFGWB notes that the intent of this qualitative study was publication in a scientific journal, not to satisfy EPA degradation study requirements.

The half-lives of irradiated pentachlorophenol at pHs 3.3 and 7.3 were 100 and 3.5 hrs, respectively. Sensitizers had no effect on the rate of photolysis. There was no degradation of pentachlorophenol in the dark controls indicating that pentachlorophenol is hydrolytically stable. The half-life of pentachlorophenol in pH 7.3 buffer irradiated with outdoor July sunlight was 48 hrs.

1. Degradates were not quantitated, thus it is not possible to establish a material balance. A valid material balance is essential to understanding and establishing the importance of aqueous photolysis in the persistence and degradation of pentachlorophenol and its degradation products. Since pentachlorophenol was not radiolabeled, and volatiles were not trapped, it is not anticipated that a material balance can be established for this study.
2. The absorption spectra of pentachlorophenol was not furnished, just the λ_{max} (320nm) was given.
3. The emission spectrum of the lamps used in the study was not furnished, nor were wavelengths <290 nm filtered

out.

4. Neither the intensity of lamp radiation or sunlight at the point of treatment was furnished.
5. The wavelength transmissibility of the borosilicate glass flasks used in the irradiation experiments was not given. Since the transmissibility of borosilicate glass varies with the manufacturing process and between manufacturers, it is not apparent what wavelengths or relative amounts of light the pentachlorophenol inside the flasks were actually exposed to.
6. No hydrolysis data were present or referred to, so the pH stability of pentachlorophenol is not known. The irradiated solutions were not sterile, so the effect of microbial degradation is not conclusively known. Also no storage stability data were given. However, the statement was made (although no data were presented) that there was no degradation of pentachlorophenol in the dark controls. Valid dark control data showing no degradation of pentachlorophenol would satisfy the above data requirements (within #6) except for pH.
7. An aqueous photolysis study was not conducted at pH 9. Studies should be conducted at the most hydrolytically stable pH of the active ingredient. In the absence of that data the aqueous photolysis study should be conducted at pHs of 5, 7, and 9.
8. The Pentachlorophenol Task Force is reminded that FIFRA requires that the registrant possess or have access to the raw data used in or generated by studies.

MATERIALS AND METHODS:

Pentachlorophenol was prepared by recrystallization three times from benzene. Aqueous 100 ppm solutions were prepared using distilled water, filtered rice-field water (a sensitizer source), and Carmody wide-range (citrate-borate-phosphate) buffers. No cosolvents were used. Irradiation vessels were borosilicate glass flasks. Neither the solutions or flasks were sterile. Radiation sources were six unfiltered F40BL lamps (spectral emission not specified) and July sunlight at Davis, California. Neither lamp or sunlight intensities at the point of treatment were given. Vessel temperatures were maintained at $26 \pm 1^\circ\text{C}$. Dark controls were run concurrently.

Four of the nine pentachlorophenol photodegradation products (tetrachlorohydroquinone, tetrachlororesorcinol, tetrachlorocatechol, and 2,3-dichloromaleic acid) were irradiated at pH 7.3 and 26°C . 2,3-dichloromaleic acid was irradiated with F40BL lamps. It was not stated what the other three photodegradates were irradiated with.

Samples of solutions were taken at the following times:

- pH 3.3 - pentachlorophenol: After 21, 50, 71, and 95 hrs of lamp irradiation.
- pH 7.3 - pentachlorophenol: Five between 0 and 10 hrs of lamp irradiation.
- pentachlorophenol: After 2, 4, 6, and 8 days of July sunlight.
- tetrachlorocatechol: After 0, 2, and 4 hrs of unknown irradiation.
- tetrachlorohydroquinone: After 0, 0.5, 1, and 2 hrs of unknown irradiation.
- 2,3-dichloromaleic acid: After 0, 25, 50, 75, and 100 hrs of lamp irradiation.

Analysis of samples was by gas chromatography; thin-layer chromatography; and infrared, ultraviolet, and nuclear magnetic resonance spectroscopy.

Test materials were not radiolabeled, volatiles were not trapped, it was not mentioned how long the samples were stored, nor were storage stability data for pentachlorophenol or its photodegradates provided.

REPORTED RESULTS:

The half-lives of UV-irradiated pentachlorophenol at pHs 3.3 and 7.3 were 100 and 3.5 hrs, respectively. It was stated that the photodegradation rates in filtered rice-field water (a source of sensitizers) and in the presence of tryptophan (a sensitizer) were the same as in distilled water, indicating that photosensitization is not a factor. No degradation of pentachlorophenol in the dark controls was reported. The half-life of pentachlorophenol in pH 7.3 buffer irradiated with outdoor July sunlight was 48 hrs (total elapsed).

The gas chromatogram of the acidic photolysis products at 50% breakdown of pentachlorophenol, showed 10 peaks. Four were irradiated. The half-lives of tetrachlorocatechol, tetrachlororesorsinol, tetrachlorohydroquinone, and 2,3-dichloromaleic acid, at pH 7.3, were approximately 2.2, 1.3, 0.2, and 48 hrs, respectively. The irradiation sources of the three former breakdown products were not given, the latter was F40BL lamps.

The proposed chemical identities of the peaks were presented (Table II) and a photodegradation scheme for pentachlorophenol was proposed (Figure 7).

DISCUSSION:

EFGWB notes that the intent of this qualitative study was publication in a scientific journal, not to satisfy EPA degradation study requirements. This undoubtedly is the reason that pentachlorophenol was not radiolabeled, volatiles were not

trapped, the emission spectrum of the lamps was not characterized nor compared or standardized to sunlight, or the degradates quantitated. The authors of the study presented largely qualitative data, EPA requires quantitative data. It is unlikely that a report which satisfies the 161-2 degradation requirements could be assembled from the raw data.

EFGWB recommends that a new study be submitted.