Dechlorination Process of Chlorobiphenyl by Light

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Introduction

Chlorobiphenyls (CBs) are organohalogen compounds shown in Figure 1 together with the numbering system at the positions on the benzene rings where chlorine atoms can be substituted. There are 209 compounds by differing in the number (from mono to deca) and position (*ortho*, *meta* and *para*; 2, 2', 3, 3', 4, 4', 5, 5', 6 and 6') of the chlorine atoms. The congener groups and number of compounds are shown in Table 1.

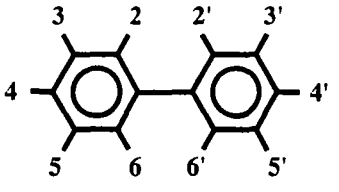


Figure 1. Basic structure of CB.

Table 1. Number of compounds for CBs.

congener	number of compounds
mono	3
di	12
tri	24
tetra	42
penta	46
hexa	42
hepta	24
octa	12
nona	3
deca	1
total	209

In the environment, the behavior of each CB compound is controlled by its physicochemical properties, and is disseminated to all matrices of the environment. In order to determine the environmental behavior of CB's, an understanding of the dechlorination and degradation processes is critical. To clarify the behavior and environmental fate of CB, obtaining accurate data regarding the dechlorination process of CB is indispensable.

This report presents data regarding the dechlorination of CB using each individual CB compound and HRGC/HRMS analysis.

Experimental Methods

For this study, all 209 CB standards and non-chlorinated biphenyl were prepared from AccuStandard (USA) and Dr. Ehrenstorfer (Germany). Each CB isomer was diluted with multi-distilled decane. 40pg/μL solutions were prepared for each isomer. Sample solutions were put into 2mL quartz container and irradiated with UV (400W, 65 μW/cm^2 at 254nm). UV irradiation experiments were carried out on a turntable that was placed in a chemical hazard clean room where room temperature was maintained at 20 ± 0.5°C. Following UV irradiation, using a digital syringe 50μL of each sample was removed and analyzed by HRGC/HRMS [1]. Samples were spiked with ^{13}C internal standard surrogates. Control samples, non-chlorinated biphenyl's, and samples not irradiated by UV were also analyzed in order to confirm the basic structure of decomposed CB and the extent of dechlorination of CB's when not irradiated with UV. A schematic diagram for this experiment is shown in Figure 2 together with the energy distribution of the UV lamp used in this experiment.

Results

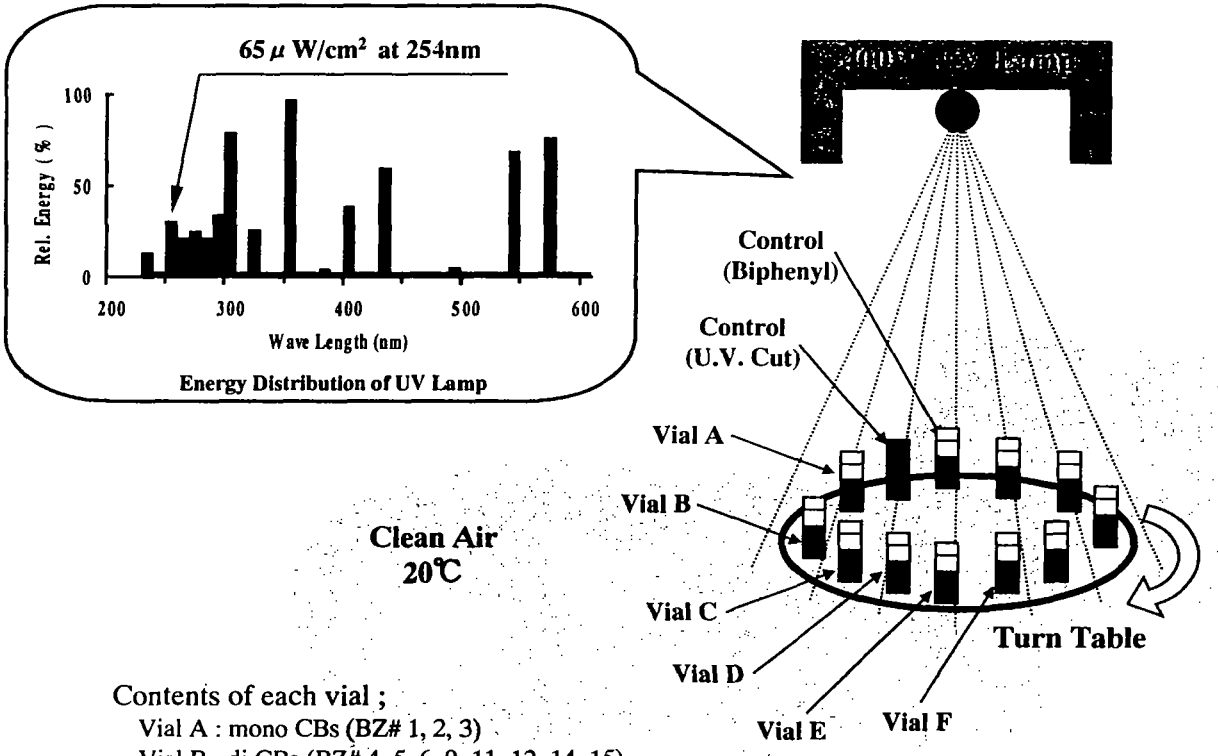
In this paper, the results for mono, di, and tri are presented. Plots of CB concentration versus UV irradiation time are shown in Figures 3,4, and 5, respectively. The decomposition of the biphenyl's basic structure was not observed in the experiment period.

Results obtained are shown;

1. Dechlorination rates of *ortho* positions (2, 2', 6, 6') are faster than other positions.
2. Dechlorination rates of *meta* (3, 3', 5, 5') and *para* (4, 4') positions are not so different.
3. Dechlorination rates of each position are controlled by not only position but also number.
4. Basic structure of biphenyl is stable for light. (Not shown in Figure)
5. Transitions of Cl atoms were observed, but effect was low. (Not shown in Figure)

Literature Cited

(1) Matsumura,T., Tsubota,H., Ikeda.Y., Chisaki,Y., Ito,H. and Morita,M.(1997) Retention order of all 209 Chlorobiphenyl compounds on capillary column SGE HT8. *Organohalogen Compounds*, 1997, **31**, 14-19.



Contents of each vial ;
Vial A : mono CBs (BZ# 1, 2, 3)
Vial B : di CBs (BZ# 4, 5, 6, 9, 11, 12, 14, 15)
Vial C : di CBs (BZ# 7, 8, 10, 13)
Vial D : tri CBs (BZ# 17, 20, 23, 24, 25, 29, 30, 32, 33)
Vial E : tri CBs (BZ# 16, 18, 19, 21, 22, 26, 27, 28, 31, 34, 35, 36, 37, 38, 39)
Vial F..... : tetra, penta, ..., and deca CBs. Results are not shown in this article.

Figure 2. Schematic diagram for the experiment.

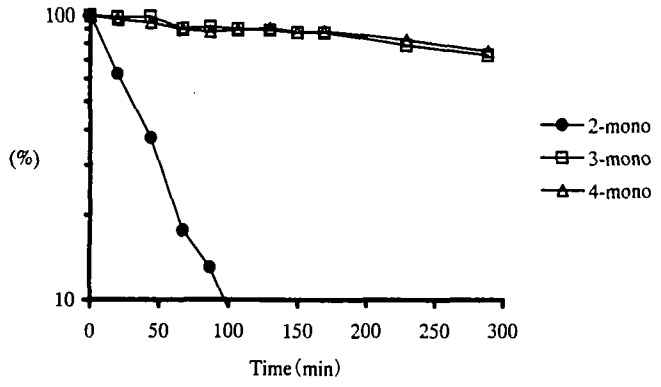


Figure 3. Concentration vs. irradiation time for mono CBs.

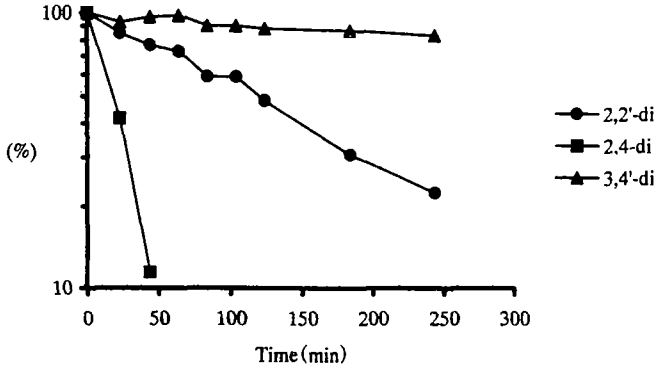


Figure 4. Concentration vs. irradiation time for di CBs.

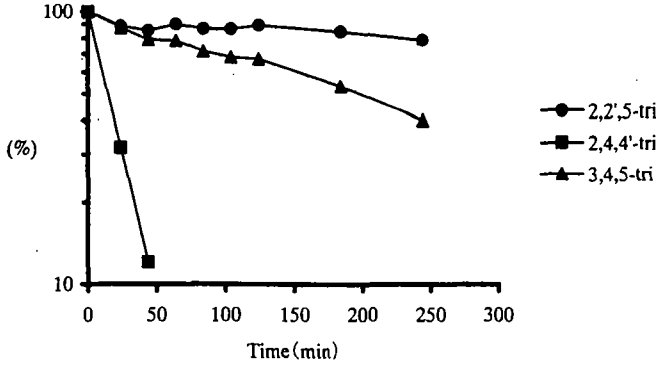


Figure 5. Concentration vs. irradiation time for tri CBs.