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Phototransformations of Polychlorobiphenyls in Brij 58 Micellar Solutions

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Our purpose in conducting these studies was to examine photolysis as a destructive process for polychlorobiphenyls (PCBs) extracted from soils with surfactant solutions. Surfactants have shown promise as agents for removing free phase and sorbed contaminants from soils, yet information on ultimate disposal options and recycle/recovery strategies for the surfactants is generally lacking. For arylhalides, photodechlorination may result in decontamination, eliminating the need to physically separate these contaminants from the washing solution. Photochemical reactions of the PCB congener mixture, Aroclor 1254, and the specific congener, 2,3,4,5-tetrachlorobiphenyl (2,3,4,5-TeCB), were investigated in aqueous solutions containing surfactant micelles with UV light at 253.7 nm. Photoreduction through photodechlorination was shown to be the main decay pathway in which lesser chlorinated congeners were formed as intermediates. In experiments with 2,3,4,5-TeCB, final noncarbon-containing products included Cl^- and H^+, both produced nearly stoichiometrically from the starting materials. The quantum yield for decay of 0.1 μM 2,3,4,5-TeCB in 0.5 mM Brij 58 micellar solutions was over six times greater than in water alone. Sequential extraction from a soil and photoreduction of 2,3,4,5-tetrachlorobiphenyl by Brij 58 solutions proved to be limited by surfactant loss to the soil.

Introduction

In a previous paper, we examined the facile nature of photodechlorination reactions of chlorobenzenes exposed to 254 nm ultraviolet light at room temperature and pressure in aqueous solutions containing surfactant micelles (*1*). In this paper, we extend this work to examine similar reactions of Aroclor 1254 and the specific congener 2,3,4,5-tetrachlorobiphenyl (2,3,4,5-TeCB). Our purpose in conducting these studies is to examine photolysis as a destructive process for arylhalides extracted from soils with surfactant solutions. Many studies have examined solubilization and/or mobilization of free phase or sorbed contaminants by surfactants in ex situ soil-washing or in situ pump-and-treat operations (*2, 3*). However, little information exists on ultimate disposal options and recycle/recovery strategies for the surfactant(s). Our hypothesis is that if surfactants are used in soil-washing and pump-and-treat technologies to assist the solubilization of arylhalide contaminants (*1, 4, 5*), photodechlorination may result in arylhalide decontamination, eliminating the need to separate these contaminants physically from the washing solution.

It is well established that many aryl halides undergo photochemical homolysis to generate aryl and halogen radicals (*6*−*8*). Bunce et al. (*8*) deduced that halogen substituents on the aromatic rings increase intersystem crossing, resulting in higher observed decay rates for the more substituted aryl (Ar) halides. Accordingly, the following mechanism was proposed, in which, upon absorption of light, ArCl produces the singlet excited state, ^{1}ArCl, which through intersystem crossing (ISC) gives the triplet, ^{3}ArCl, which upon dissociation produces the aryl radical, Ar$^\bullet$, and a chlorine atom, Cl$^\bullet$.

$$\mathrm{ArCl} \xrightarrow{h\nu} {}^1\mathrm{ArCl} \xrightarrow{\mathrm{ISC}} {}^3\mathrm{ArCl} \rightarrow \mathrm{Ar}^\bullet + \mathrm{Cl}^\bullet \qquad (1)$$

Bunce et al. (*8*) found that, in isooctane at 254 nm, ortho-chlorinated biphenyls were more photolabile than non-ortho-chlorinated biphenyls, presumably because of increased efficiency in intersystem crossing leading to the triplet state, and a reduced half-life of the triplet state due to a steric effect. From a remediation standpoint, this is significant as ortho-chlorines tend to be more recalcitrant to anaerobic dehalogenation.

In the presence of hydrogen sources or other electron donors, the reaction also may proceed through an electron-transfer process. In the electron-transfer process, the donor molecule furnishes an electron to the excited aryl chloride (ArCl*), forming an unstable aryl radical anion which cleaves to form the aryl radical and chloride.

$$\mathrm{D} + \mathrm{ArCl}^* \rightarrow \mathrm{D}^{\bullet+} + \mathrm{ArCl}^{\bullet-} \rightarrow \mathrm{Cl}^- + \mathrm{Ar}^\bullet \xrightarrow{\mathrm{R-H}} \mathrm{ArH} \quad (2)$$

As in homolysis, cleavage of the C−Cl bond forms an aryl radical, which may abstract hydrogen from the hydrogen donor, forming the product ArH.

Freeman and coauthors (*9*−*11*) further defined three subpathways within this general mechanism: singlet fragmentation, fission of the triplet, and fragmentation via the triplet excimer. In the case of pentachlorobenzene, photolysis in CH_3CN at 254 nm gave 1,2,3,5-tetrachlorobenzene as a major product along with 1,2,4,5-tetrachlorobenzene and 1,2,3,4-tetrachlorobenzene as minor products. This was proposed to occur mainly by way of the triplet and triplet excimer pathways with a minor contribution (2−6%) from the direct fission of the singlet. In the presence of the electron donor, triethylamine, a reversal in the regiochemistry occurs, such that 1,2,4,5-tetrachlorobenzene is formed as the major product due to the generation of pentachlorobenzene radical anions through the transfer of an electron from triethylamine to pentachlorobenzene. A similar reversal in regiochemistry occurred when the reaction was carried out in 200 mM hexadecyltrimethylammonium bromide (CTAB) with 165 mM triethylamine, presumably with a portion of the triethylamine residing near the surface of the CTAB micelles, with pentachlorobenzene concentrated within the micelles.

Few photochemical studies with chlorinated biphenyls have been conducted in micellar solutions. Epling et al. (*12*) reported quantum yields of about 0.1 for 4-chloro- and 4,4′-dichloro-biphenyl in highly concentrated solutions (130 mM)

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of Brij 58, both approximately 100-fold greater than in 9:1 acetonitrile−water mixtures. This suggests that similar enhancements may occur for other congeners.

However, for photolysis to be a feasible destructive process for arylhalides extracted with surfactants from soils, information regarding surfactant reuse or recovery and quantum yields for decay in these complex systems must be known. Previously, we and others have shown that precipitation (*13*) and sorption (*14*) are processes that control recovery of anionic and nonionic surfactants, respectively, from aqueous slurries of some typical North American soils. In the latter case, it was shown that sorption of polyethoxyated alcohol surfactants increased with increasing polyethoxy chain length within a homologous series of linear ethoxylated alcohols. Sorption isotherms display plateau maxima at aqueous concentrations exceeding the critical micelle concentration (cmc) due to micelle formation. At surfactant doses sufficient to form micelles, the aqueous phase of soil−water slurries often is quite colored due to solubilization of humic material. The effect of these materials on quantum yields in micellar solutions has not previously been investigated.

The purpose of this study was to survey the reactivity of Aroclor 1254 in various mixtures containing micelles of the nonionic surfactant Brij 58, to investigate the photodechlorination patterns of 2,3,4,5-TeCB in similar micellar solutions, and to test the reactivity of 2,3,4,5-TeCB after its extraction from contaminated soils with Brij 58.

Materials and Methods

Chemicals. All solvents were HPLC grade, purchased from Fisher, Mallinckrodt, or Aldrich. 2,3,4,5-Tetrachlorobiphenyl (2,3,4,5-TeCB) and 4-chlorobiphenyl (4-CB) were purchased from Aldrich and used without further purification. Sodium borohydride (SBH) (99%), purchased from Aldrich, was often added as an additional electron donor. All solutions were prepared with distilled water, made by distilling deionized water which contained 0.01 M $KMnO_4$ and 0.01 M KOH added to the still to oxidize organic impurities. Brij 58 ($C_{16}H_{33}(OCH_2CH_2)_{20(ave)}OH$) was purchased from Aldrich Chemical Co. and used without further purification. As with other formulations of nonionic ethoxylated surfactants, Brij 58 is a mixture of homologues containing various ethoxy chain lengths.

Methods. All photochemical experiments were conducted within a RPR-100 Rayonet photochemical reactor equipped with a merry-go-round apparatus (Southern New England Ultraviolet) placed in a dark room. All solutions were illuminated in cylindrical quartz cuvettes placed within the merry-go-round. Light sources were two 253.7 nm phosphor-coated low-pressure mercury lamps (Rayonet). The light intensity within each tube was determined from separate tubes containing the chemical actinometer, potassium ferrioxalate (*15*). The zero-order decay product, $Fe(C_2O_4)_2^{2-}$, was determined spectrophotometrically upon Fe(II) complexation with 1,10-phenanthroline. The number of photons entering each tube per unit volume per unit time, $I_{\lambda=254.7}$ (*16*), was generally about 5.6×10^{-6} einstein L^{-1} s^{-1}.

In each experiment, 5 mL aqueous solutions each containing identical concentrations of 2,3,4,5-TeCB or Aroclor 1254, Brij 58, and often SBH and/or NaOH were irradiated in the photoreactor. Tubes were removed as a function of time with the concentration at time 0 determined from analysis of an unexposed sample to which SBH was not added. The initial experimental stock solutions of 2,3,4,5-TeCB were saturated solutions in water or the surfactant solution, centrifuged to remove excess solid phase. Stock solutions of the Aroclor were centrifuged and water-saturated. No additional solvents were introduced.

Compounds and products were extracted into isooctane prior to analysis. To avoid the formation of emulsions in the extraction step, 4 mL of each illuminated sample was transferred to a 25 mL test tube, diluted with approximately 10 mL of distilled water, and carefully overlaid with 2 mL of isooctane. Tubes were gently agitated just slightly off vertical with a twist-action shaker in the dark at 20 °C for 24 h. With this method, the extraction efficiency of each PCB congener was determined to be approximately 100%.

PCBs were quantified with a Hewlett-Packard 5890 Series II gas chromatograph (GC) equipped with a splitless injector, an electron capture detector (ECD), an integrator, and a 28 m × 0.323 mm DB-5 column (film thickness of 0.25). In experiments with 2,3,4,5-TeCB, the molecular masses of products were determined by GC-MS analysis with a Finnigan MAT 800 mass spectrometer and HP 5890A GC equipped with the same length and diameter DB-5 column as that used for product quantification. Relative retention times of ECD-sensitive species were compared to those reported by Mullin et al. (*17*) to further confirm identifications, with the measured retention times of 2,3,4,5-TeCB and 4-CB used as calibration points. For this purpose, the GC temperature was ramped from 100 to 220 °C at a rate of 2.2 °C/min. Approximate yields of products were estimated from the relative response factors (*17*). For analysis of Aroclor 1254, the GC temperature was ramped from 65 °C (for 2 min) to 200 °C at a rate of 30 °C/min, to 250 °C at a rate of 2 °C/min, and to 300 °C (for 2 min) at a rate of 30 °C/min. In some experiments, chloride was determined with a Dionex 2000i/SP ion chromatograph, equipped with an Ion Pac AS4A 4 mm chromatographic column and conductivity detector. The mobile phase was a carbonate−bicarbonate buffer (2.8 mM $NaHCO_3$ and 2.3 mM Na_2CO_3). pH was measured with a Fisher Scientific Accumet 925 pH/ion meter and a general purpose Orion glass Ross combination electrode.

Initial decay rates of 2,3,4,5-TeCB were determined from the integrated first-order decay expression

$$P_t = P_0 e^{-k_p t} \tag{3}$$

where P_0 and P_t are the concentrations of the 2,3,4,5-TeCP at time 0 and t, respectively, and k_p is the first order decay rate constant (s^{-1}). The quantum yields with the monochromatic light source were calculated from k_p and the light intensity by (*16*)

$$\Phi_P = \frac{k_p}{2.303 I_{\lambda,0} \epsilon_{p,\lambda} l} \tag{4}$$

where Φ_P is the quantum yield, $I_{\lambda,0}$ is the light intensity term (einstein L^{-1} s^{-1}) (*16*), $\epsilon_{p,\lambda}$ is the molar absorptivity at 254 nm (L mol^{-1} cm^{-1}), and l is the cell path length term (cm).

In a final experiment, two samples of a soil, designated EPA-11 (*18*) were contaminated with 0.58 and 1.4 mmol of 2,3,4,5-TeCB/kg of soil by plating the compound on the walls of glass containers (upon volatilization of the solvent carrier) and mixing dry soil samples with water (1:10 soil mass to volume) in the containers for 48 h. Subsamples (5.0 and 0.5 g) of the 0.58 and 1.4 mmol/kg contaminated samples, respectively, were extracted with 100 mL of water containing 1 mM Brij 58 for 4 h and centrifuged at 10 000 rpm for 10 min. The aqueous solutions were illuminated in the photoreactor for three minutes, measuring the concentration of 2,3,4,5-TeCB before and after illumination by extracting 2 mL of the solution with isooctane. This procedure was repeated several times, each time using the same illuminated solution to extract the solute from a new 5.0 or 0.5 g soil subsample.

Results and Discussion

Aroclor 1254 Photodecay. Aqueous saturated solutions of Aroclor 1254 containing as additives 0.5 mM Brij 58, 50 mM

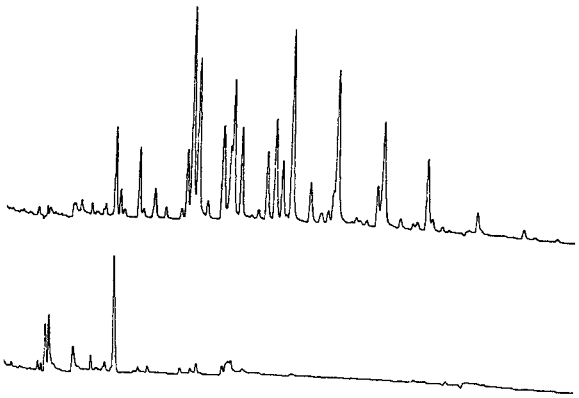

FIGURE 1. Photodecay of Arochlor 1254 in a Brij 58 micellar solution. Arochlor 1254 GC trace before (top) and after (bottom) 5 min of illumination at 253.7 nm. An aqueous saturated Arochlor 1254 was used. The light intensity was 5.7 × 10^{-6} einstein s^{-1} L^{-1}.

SBH, and/or 10 mM NaOH were illuminated in the photochemical reactor for 24 min. The combination of additives was (1) water only, (2) Brij 58 only, (3) Brij 58 and SBH, (4) Brij 58 and NaOH, (5) SBH and NaOH, and (6) Brij 58, SBH, and NaOH. Small volumes of each additive were combined with the aqueous saturated solution of Aroclor 1254. After 24 min of illumination of sample 1 (water), about 15% of the PCB peaks (by ECD), by number and area, remained, whereas in the presence of Brij 58 (sample 2), only one peak was evident. Samples with Brij 58 and SBH (sample 3), Brij 58 and NaOH (sample 4), and Brij 58, SBH, and NaOH (sample 6) resulted in no quantifiable peaks by the ECD. For sample 5 (SBH and NaOH), however, approximately 6% of the total area remained on the chromatograph, despite the addition of the strong base-stabilized reducing agent. Qualitatively, Brij 58 at 0.5 mM was more effective than 50 mM SBH in facilitating the overall reactions.

Sample GC traces of the Aroclor before and after illumination are shown in Figure 1. This particular sample contained 0.5 mM Brij 58, and the sampling time was 5 min. Evident on the illuminated trace is the disappearance of higher molecular weight homologues, the appearance of peaks with shorter retention times, and the increased peak areas of some lower molecular weight homologues.

Kinetic experiments were performed with Aroclor 1254 with these same additives. Relative peak areas for the 17 most prominent congener or coeluting congener peak areas are shown in Figure 2 for solutions containing (1) water only, (2) 0.5 mM Brij 58, and (3) 0.5 mM Brij 58, 50 mM SBH, and 10 mM NaOH, after 0, 1, 3, and 24 min illuminations. The addition of Brij 58 with or without SBH enhanced the total rate of decay. The formation and decay of some of the lower chlorinated biphenyls (shorter retention times) is a direct indication that the higher chlorinated biphenyls at longer retention times are undergoing photodechlorination.

2,3,4,5-TeCB Photodecay. 2,3,4,5-TeCB was chosen as a representative congener for more quantitative studies. Upon illumination of 6.1 μM 2,3,4,5-TeCB containing 2.0 mM Brij 58, the chloride ion concentration increased from 0.74 to 27 μM within 60 min. During the same time period, the pH of the reaction mixture decreased from 7.03 to 4.56. Assuming unity activity coefficients to calculate proton ion concentrations and no buffer capacity of the solution, the formation of chloride and proton ions matches nearly stoichiometrically.

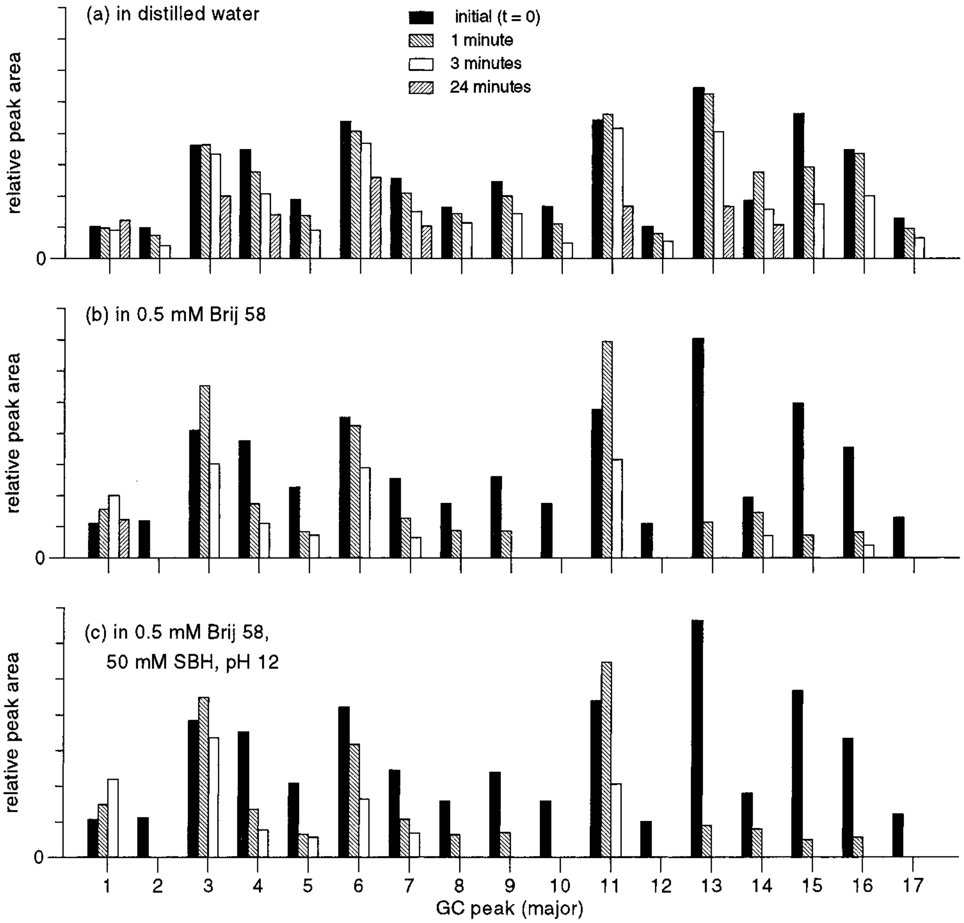

FIGURE 2. Photodecay of Arochlor 1254 with various additives. Brij 58 (5.0 × 10^{-4} M), SBH (0.05 M), and NaOH (0.01 M) were used as additives to a saturated Aroclor 1254 solution. The cell path was 1.0 cm. Peak number indicates order of retention time from short to long.

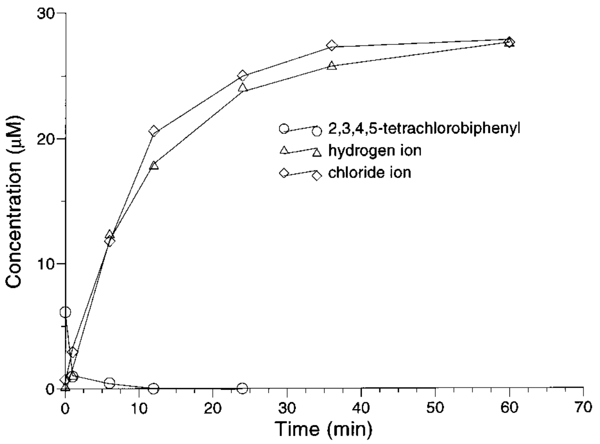

FIGURE 3. Photodecay of 2,3,4,5-TeCB in Brij 58 micellar solution. Initial concentrations were 2.0 × 10^{-3} M Brij 58 and 6.1 × 10^{-6} M 2,3,4,5-TeCB. The cell diameter was 1.3 cm.

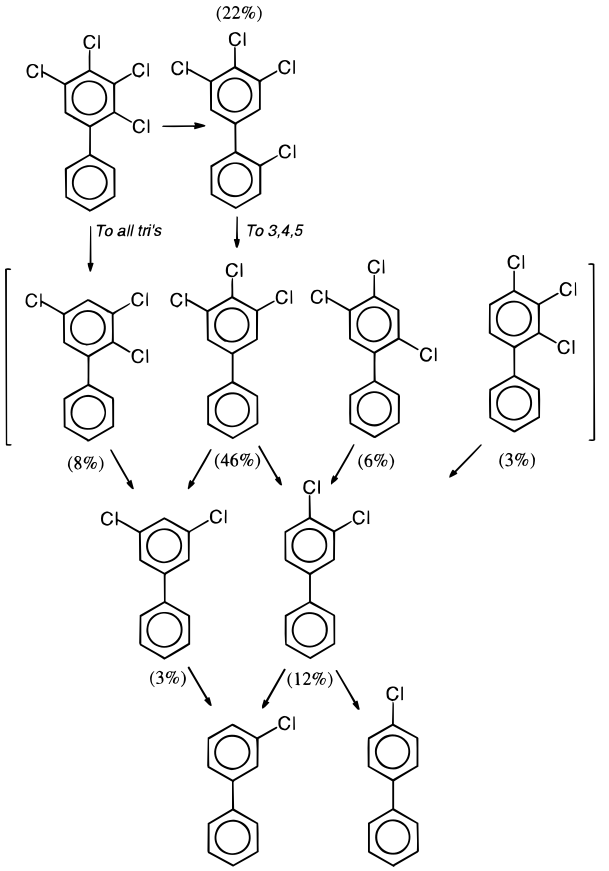

FIGURE 4. Decay pathway of 20 μM 2,3,4,5-TeCB in 0.5 mM Brij 58 solutions. Numbers in parentheses indicate percent yield at 30 s with a light intensity of approximately 5.7 × 10^{-6} einstein s^{-1} L^{-1}. The monochlorobiphenyls are observed at later times.

The photodecay of 2,3,4,5-TeCB and the formation of Cl^- and H^+ with time are shown graphically in Figure 3. Over this time period, 10 peaks appear and most disappear on the chromatrograms. All peaks were identified by GC−MS analysis and relative retention times (RRTs) to be congeners with the following substitution patterns: 2′,3,4,5-, 2,3,4,5-, 3,4,5-, 2,3,4-, 2,4,5-, 2,3,5- or 2′,3,5-, 3,4-, 3,5-, 4-, and 3-. From this information, the decay pathway shown in Figure 4 is proposed. The percent yield values indicated by each congener on this figure are those relative to the total molar concentration of chlorinated products observed at 30 s for a 20 μM 2,3,4,5-TeCB, 0.5 mM Brij 58 solution. About half of the orginal 2,3,4,5-TeCB is decayed at this point, with nearly stoichiometric recovery of the remaining as chlorinated products. The photoreactivity of the ortho-chlorine in organic solvents is well documented (see refs *6*−*8*), so it is not surprising that the majority of the parent compound decays to 3,4,5-trichlorobiphenyl (3,4,5-TriCB). The data indicate that this intermediate is reached through two pathways. The first may occur either by homolysis, forming a biphenyl radical, which may abstract a hydrogen from the surfactant hydrocarbon, or possibly by the triplet excited state abstracting a hydrogen from the surfactant hydrocarbon. Both mechanisms result in photodechlorination and formation of the chlorine radical, which likely abstracts an electron or H-atom from the surfactant, forming the observed chloride ion product.

The second pathway leads to an overall 1,4-shift isomerization reaction, forming 2′,3,4,5-TeCB in high yields; whether radical separation occurs is unknown. To our knowledge, this specific isomerization reaction has not previously been reported. Isomerization of chlorinated benzenes has been observed previously in aqueous micellar (*1*), methanolic (*19*), and aqueous acetonitrile (*20*) solutions.

Many studies in homogeneous nucleophilic solvents (i.e., CH_3OH) indicate that dimerization reactions may occur, but indication of these products was not evident. This was anticipated on the basis of the low occupancies of the PCB congeners in the micelles that occur at the PCB−surfactant ratios employed in this study, and because of the greater hydrogen-donating ability of the surfactant compared to methanol. With on average less than one congener per micelle, the reactive aryl free radicals are likely isolated from each other in restricted space.

The decay quantum yield of 0.1 μM 2,3,4,5-TeCB was determined in solutions of (i) distilled water, (ii) 0.5 mM Brij 58, and (iii) 0.5 mM Brij 58, 50 mM SBH, and 10 mM NaOH and found as 0.034, 0.21, and 0.24, respectively. These values are based on the measured 2,3,4,5-TeCB molar absorptivity of 8630 L mol^{-1} cm^{-1} at 254 nm in isooctane. The inability of SBH to significantly enhance the rate above that of Brij 58 alone is not entirely surprising as the affinity of BH_4^- for the hydrocarbon core of the micelle, where the excited state 2,3,4,5-TeCB is most likely located, is very low.

Soil Washing. The results of a series of extractions and illuminations, using the same Brij 58 solution each time as the extracting agent on a new subsample of the contaminated soil, are displaced graphically in Figure 5. When a 0.5 g/100 mL soil solution contaminated with 1.4 mmol/kg 2,3,4,5-TeCB was used, over 80% of the 2,3,4,5-TeCB was recovered from each subsample (≈5.8 μM) for the first three serial extractions. A previous study with a historically contaminated sediment showed that increased mass recovery of PCB congeners is possible by performing serial extractions on the same soil (*4*). Once extracted, the 2,3,4,5-TeCB was dechlorinated to less than 10 nM in less than 3 min of irradiation. This time was not sufficient to dechlorinate reaction products, although longer irradiation times could have been used for this purpose. After three cycles, no loss in extraction or photolysis efficiency was observed; however, the fourth cycle showed loss of extraction efficiency, most likely due to surfactant adsorption to the soil. Absorbance of the solution at 254 nm increased after each cycle, indicating accumulation of humic material in the reused micellar solution.

In a separate experiment, we irradiated 2,3,4,5-TeCB in solutions containing Brij 58 and material extracted from soil with this surfactant, having light absorbances at 254 nm of about 0.5, and measured quantum yields equal to or slightly exceeding those in similar solutions containing Brij 58 alone. It is likely that light attenuation due to these materials at this

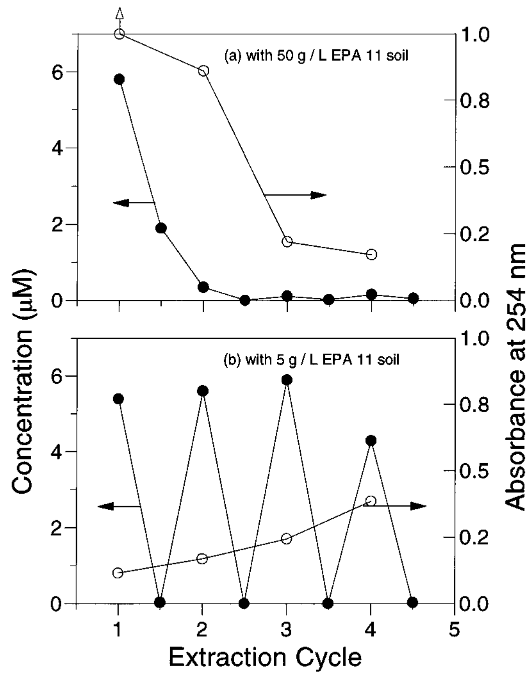

FIGURE 5. Photolysis of 2,3,4,5-TeCB (left scale) extracted from EPA-11 soil with 1 mM Brij 58, with reuse of the surfactant solution. The absorbance at 254 nm (right scale) increases with each reuse.

absorbance is offset by increased indirect or sensitized photolysis.

Contaminating the soil with 0.58 mmol of 2,3,4,5-TeCB/kg of soil, and extracting 5 g of this soil with 100 mL of water containing 1 mM Brij 58, results in a concentration of 2,3,4,5-TeCB similar to that in the above case. However, as shown in Figure 5a, the light absorbance of this solution at 254 nm exceeded 2.0, and illumination for 3 min was not sufficient to dechlorinate the congener due to optical inhibition. The second serial extraction resulted in readsorption of the congener rather than extraction and a decrease in light absorption, both indicating the absence of micelles. At this soil concentration, loss of Brij 58 homologues to the soil matrix inhibits effective contaminant extraction, yet excessive extraction of humic materials inhibits photodechlorination.

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