An experimental study of photodegradation of bisphenol A in water: Reaction with hydroxyl radical

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Introduction

Solar irradiation can cause degradation of organic pollutants in surface natural waters via direct and indirect photoreactions. Hydroxyl radical (•OH) is one of the transient in photochemical process and is the most oxidative reactant among free radical species. The primary source of •OH in most surface natural waters is nitrate photolysis (Zepp et al., 1987).

We present here the photodegradation of the estrogen-like pollutants, bisphenol A due to its reaction with •OH initiated by nitrate photolysis in water.

Results and disccsion

After light irradiation using the solar simulator, the concentration of bisphenol A was determined in water containing nitrate. In the absence of nitrate, the result of little degradation of bisphenol A suggests that direct photoreaction of bisphenol A is insignificant under sunlight exposure. In the presence of nitrate, where •OH are formed, faster degradation of bisphenol A was observed as compared to direct photoreaction. However, concentrations of dissolve organic carbon (DOC) were constant during irradiation experiment (Figure 1). These results indicate that degradation of bisphenol A is caused by nitrate photolysis and suggest that bisphenol A is transformed to other organic compounds.

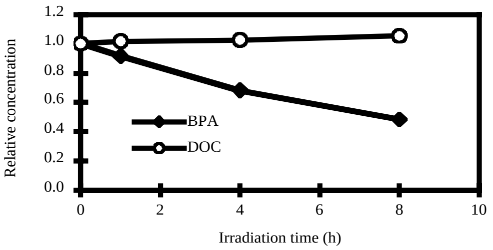

Figure 1. Bisphenol A (BPA) and dissolved organic carbon (DOC) concentration upon irradiation time. Initial concentration of BPA, DOC and nitrate were 1.15 mg L^{-1}, 1.13 mg L^{-1} and 1 mmol L^{-1}.

The solution containing the photodegradated bisphenol A showed less inhibitory effects on steroidogenesis with bisphenol A than non-degradated solution. It indicates that photo-induced transformation of bisphenol A with hydroxyl radical reduced the hormonal activity of bisphenol A. We will also present the products from the reaction of bisphenol A with •OH.

References

Zepp et al. (1987) Environ. Sci. Technol. 21, 443-450.

An interpretation of ^{11}B and ^{29}Si NMR spectra in alkali borosilicate glasses

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Alkali borosilicate glasses have wide variety both in chemical and physical properties, so they have been widely used as commercial glasses. Several structural models have been proposed for the alkali borosilicate glasses. The authors have also investigated the glass structure by means of spectroscopic metods, such as XPS, ^{11}B and ^{29}Si NMR, in which conflicts were found among the experimental results. The amounts of alkali oxide consumed to form BO_4 units (R_{B4}) and NBO in SiO_4 units (R_{Si}) are determined from ^{11}B NMR and ^{29}Si NMR, respecticely, and the amount for the formation of NBO in BO_3 units (R_{B3}) are also estimtated from R_{B4} and R_{Si}. As shown in Figure 1, R_{B4} decreases and R_{Si} increases with increasing the total Na_2O content R, and R_{B3} however shows negative value in the small R region, indicating the conflict between ^{11}B and ^{29}Si NMR, that is, an overestimation of NBO in ^{29}Si NMR. It was therefore assumed that a part of bridging oxygens (BOs) in B–O–Si bonds had been originally NBOs in SiO_4 units and they possessed much higher electronic population than the other BOs. In this paper, the assumption was verified on the basis of theoretical MO calculaions, in which some cluster models were constructed from crystalline borosilicates and electronic states of oxygen atoms were evaluated with Mulliken population analyses.

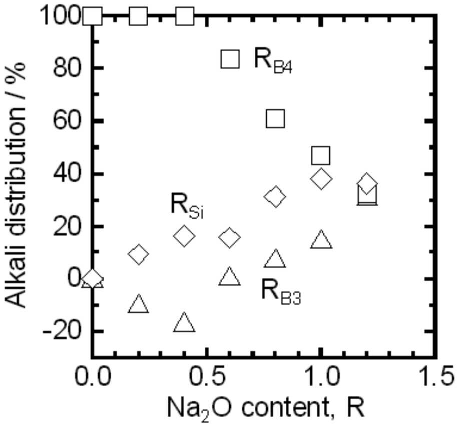

Figure 1: Relative amout of alkali oxide distributed for the formation of BO4 unit (RB4), NBO in SiO4 unit (RSi) and NBO in BO3 unit (RB3) in R Na2O·B2O3·0.5 SiO2 glass.

References

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Nanba T. and Miura Y., (2003), *Phys. Chem. Glasses* (in print).