

## Photochemical degradation of bisphenols -F, -S and -Z in aqueous solution: degradation kinetics and identification of transformation products

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Bisphenols (BPs) are high production volume industrial compounds that are used as monomers in the production of polycarbonate and epoxy resins for food contact materials and as developers in thermal paper. In recent years, extensive research has been performed to assess the toxicity of bisphenol A (BPA), which was the most applied BP. Because of its classification as an endocrine disruptive compound and following regulations on its production and use, BPA is being replaced by other BPs in aforementioned applications. These BPA analogues have been detected in humans and in the environment. Because of their structural similarity to BPA, BPs potentially exert similar toxic effects and therefore, it is important to study their occurrence and fate in the environment.

Recent studies have reported the photochemical degradation of various BPs. In this study, 4-[(4-hydroxyphenyl)-methyl]phenol (bisphenol F, BPF), 4-(4-hydroxyphenyl) sulfonylphenol (bisphenol S, BPS) and 4-[1-(4-hydroxyphenyl)cyclohexyl]phenol (bisphenol Z, BPZ) were exposed in aqueous solution to monochromatic UV light ( $\lambda_{\max} = 254 \text{ nm}$ ) with an intensity of  $8.91 \times 10^7 \text{ Einstein/s}$ , using a low pressure mercury lamp. Three experiments were carried out for each BP in an immersion reactor: 1) exposure to UV light, 2) exposure to UV with addition of  $\beta$ -cyclodextrin ( $\beta$ -CD) and 3) exposure to UV with addition of  $\text{H}_2\text{O}_2$  and  $\text{Fe}^{2+}$  (photo Fenton).

First, we determined the kinetic profiles for the photochemical degradation of the three BPs and the degradation efficiency of the three different treatments. The initial concentrations of BPs were 200 ng/L in MilliQ water. After UV exposure for time intervals ranging from 10 min to 4 h, two aliquots of 350 mL were sampled and analyzed. The analytical method consisted of SPE, followed by derivatisation with BSTFA and analysis by GC-EI-MS. Degradation of the BPs under these conditions followed pseudo-first-order kinetics. Half-lives of the three compounds were shortest when the photo-Fenton reaction was applied; 16.1 min, 21.7 min and 16.5 min for BPF, BPS and BPZ, respectively.

In a second set of experiments, we have attempted to identify the major transformation products (TPs) of the BPs using initial concentrations of 5 mg/L in milliQ water. Aliquots of 1 mL were sampled in duplicate at the same time intervals and were analysed by LC-ESI-QTOF in scan mode. False positive signals were filtered out by comparing the duplicates of each sample with the signal in the blanks and with the samples at  $t = 0 \text{ min}$ . Structural elucidation and confirmation will be carried out by acquiring a MS/MS spectrum for the detected molecular features. So far, hydroxylated TPs of all three BPs have been detected, as well as products from cleavage reactions. Besides the identification of TPs, we will also examine whether the various treatments promote different photodegradation pathways.