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Method for identification of chemical stability and prediction of bioaccumulation

JOHAN ERIKSSON

ÅKE BERGMAN

Dept of Materials and Environmental Chemistry

STOCKHOLM UNIVERSITY

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Results during phase 1

The work on identification of chemical stability and prediction of active bioaccumulation has been continuously going on since the start of ChEmiTecs. This has resulted in a number of articles (1-5) and one thesis (6). The work has, based on two previous theses by Eriksson (7) and Rahm (8), led to the thesis defended by Moreira Bastos (6) on methods for environmental chemical oxidative reactivity. Further, the environmental chemical reductive reactivity has been studied and a method has been developed for assessment of this type of transformations of chemicals in the environment (4). The methodology for assessing environmental transformations of chemicals is accordingly rather complete in a first round. In fact, our studies have addressed the issue of radical reactions of anthropogenic compounds in the environment. From here we have now taken steps to start the next generation of testing procedures regarding both abiotic and biological transformations of chemicals.

The available methods for studies of chemical stability/reactivity have been applied for a set of case study chemicals, including the five phthalate ester: DMP, DEP, DnBP, BBP and DEHP plus one aromatic and frequently used phosphate ester, TPP (5). The test compound structures are shown in Figure 1 below. The study has included photolysis, hse reactivity and oxidations and the results are presented in a preliminary manuscript (5). It is clear from the lack of measurable degradation rates through photolysis and oxidations that all these substances are non-reacting compounds in relation to these transformations. In contrast all five phthalate esters are hydrolyzed under the hse conditions applied, with BBP being the most reactive and DEHP the least reactive compound. The phosphate ester, TPP was even further reluctant to hse reactions than the phthalate esters, showing no apparent rate of transformation. The ester hydrolyses are catalyzed by acid or base but the environmental conditions are rather close to neutral. Hence the results of the present study are showing high reluctance to undergo abiotic transformations, promoting the conclusion that these compounds have a high persistency.

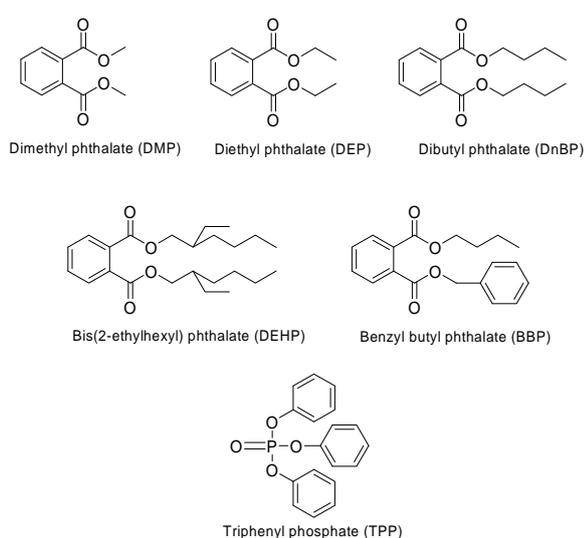


Figure 1. Structures of the the test compounds regarding chemical ractivity.

Both the phthalate esters and the phosphate ester are readily transformed biologically, reactions catalyzed by enzymes leaving them as semi-persistent chemicals. The study compounds have not yet been subjected to reductive test conditions but it is possible to state that the compounds do not reduce. One electron transfer reactions, free radical reactions, are possibly the main environmental transformation of the esters tested.

Reductive debromination of the three possible nonabrominated diphenyl congeners (BDE-206, BDE-207, and BDE-208) has been studied by a recently developed semi-quantitative method (3). The three nonabrominated DEs gave isomer-related transformation product patterns (Figure 2). As shown in this figure, all nonabrominated DEs displayed a preferred initial debromination on the fully brominated DE ring even though some minor products from debromination in the unfilled ring could be observed. BDE-207 and BDE-208 showed a propensity for *ortho*-debromination in the initial reaction step, while no discrimination between initial debromination positions was seen for BDE-206. Since the method is so far only semi-quantitative it is not possible to draw any far-reaching conclusions about their reaction rates but tentative results of the reductive debromination by sodium borohydride give similar half-lives for all the nonabrominated DEs, indicating small differences in transformation rates.

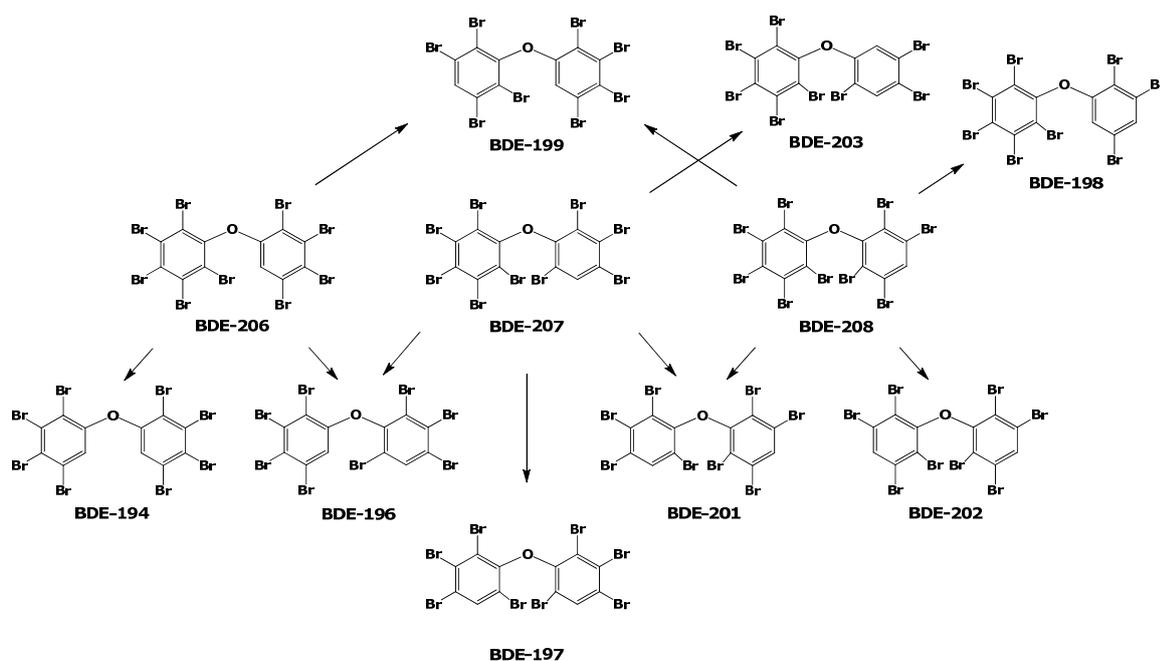


Figure 2. Reaction pathways for the reductive debromination of BDE-206, BDE-207, and BDE-208.

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