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Identification of selected polybrominated diphenyl ethers in electrical and electronic equipment and environmental samples using FTIR spectroscopy

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Polybrominated diphenyl ethers (PBDEs) are used as flame retardants in a variety of consumer products including electrical and electronic items. They have become widespread environmental pollutants due to their persistence, lipophilicity and bioaccumulating property. A study on PBDEs is important as exposure to these chemicals could result in adverse health effects such as endocrine disruption, liver toxicity, developmental toxicity, developmental neurotoxicity and reproductive toxicity.

GC/MS, GC incorporated with ECD or ECNI with capillary columns are the widely used analytical methods for the determination of PBDEs. However, these methods are expensive and time consuming. IR spectroscopic methods on the other hand are fast, simple, non destructive and cost effective. This study was focused mainly on investigating an IR spectroscopic method to identify PBDEs in electrical and electronic equipment.

Since, BDE 209 is the major congener present in c-decaBDE, it was the compound of primary interest in this project. For the identification of PBDEs by FTIR (Attenuated Total Reflectance), the fingerprint region from 1000 cm^{-1} to 1500 cm^{-1} was found to be important. Vibrational data assignment for the BDE 209 molecule was also proposed in this study.

A variety of electrical and electronic goods namely, computer mother boards, computer CPU casings, an electric switch, an electric plug, a cell phone, cell phone charger casings, a multi plug, radio casings, a wire used in a computer power supply unit were analyzed for BDE 209 using FTIR spectrometry. Further, in order to determine whether a selected environment was polluted with PBDEs, three dust samples and a soil sample were also analyzed. The IR spectrum of BDE 209 standard was compared with those of the samples, in order to determine its presence. The most prominent peaks of BDE 209 (1348, 1342, 1323, 1311, 1504, 1496 cm^{-1}) were used.

The results showed that BDE 209 was present in computer mother boards, CPU casings, an electric switch, an electric plug, a wire used in a computer power supply unit, a cell phone and radio casings. The dust sample collected from computer repair shop and the soil sample collected from e-waste recycling site were also found to have BDE 209 in small quantities. It can be concluded that IR spectroscopy is a successful analytical method for the identification of PBDEs in both polymeric and environmental samples.

Further, the IR spectrum of BDE 209 was calculated using three levels of theory namely, HF/6-31G, B3LYP/6-31G(D) and B3LYP/6-31+G(D). Good agreement between the IR spectrum of BDE 209 and the IR spectrum generated using B3LYP/6-31G(D) was obtained. IR spectra of BDE 47, BDE 99, BDE 153 and BDE 183 were also calculated using the same method, as lower BDE congeners are the predominant ones in the environment and biota.

This study shows that FTIR/ ATR could be effectively used to determine the presence of PBDEs in areas where electrical and electronic equipment is extensively used and in e-waste /dumping disposal /collecting /sites.

Keywords: e-waste, flame retardant, FTIR, PBDEs

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