Crystal structure of PCB 77 (3, 3', 4, 4'-tetrachlorobiphenyl), a dioxin-like PCB congener. (a) Molecular structure of PCB 77 showing the atom-labeling scheme and (b) view of PCB 77 along the C1–C1′ axis illustrating the non-planar conformation of the molecule. Displacement ellipsoids are drawn at the 50% probability level. Unlabeled atoms are at the symmetry position (1 – x; 1 – y; z). (Shaikh et al., Chemosphere 2008)