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Degree of phenyl chlorination of DDT-related compounds as potential molecular indicator for industrial DDT emissions

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Research highlights

- First identification of DDX with additional or missing chlorine atoms ($DDX^{\pm Cl}$)
- Detection of $DDX^{\pm Cl}$ in the vicinity of current and former DDT production sites
- Link between the production of impure technical grade DDT and $DDX^{\pm Cl}$ occurrence
- Syntheses of reference compounds to simulate production of impure technical DDT
- Assessment of $DDX^{\pm Cl}$ as molecular indicators for industrial DDT emissions

Abstract The pesticide DDT (1-chloro-4-[2,2,2-trichloro-1-(4-chlorophenyl)ethyl]benzene) and its degradates are among the most persistent and abundant organochlorine contaminates in the environment, and DDT is still being produced in several Asian countries. In this study, we report for the first time on the detection of DDT-related compounds with one additional or missing chlorine atom at the phenyl group ($DDX^{\pm Cl}$) in sediment and soil samples taken in the vicinity of former and current DDT production sites. These congeneric compounds most likely originate from production residues disposed of into the environment. In order to ensure an adequate identification and quantification of this novel organic pollutant group, individual $DDX^{\pm Cl}$ were synthesized as reference compounds by simulating an impure production of DDT in the laboratory. In contrast to $DDX^{\pm Cl}$ with (chloro)alkyl moieties, $DDX^{\pm Cl}$ with (chloro)alkenyl moieties cannot be unambiguous assigned by gas-chromatographic/mass spectrometric (GC/MS) fragmentation and elution orders. The occurrence of $DDX^{\pm Cl}$ in environmental samples allows to draw conclusions about the purity of the production process in the associated production sites. Moreover, they potentially can serve as molecular indicators to differentiate between industrial DDT emissions and insecticidal applications of DDT. This hypothesis has yet to be confirmed by further research.

Keywords DDT · production residues · deviating chlorination · GC/MS screening