

## Trixylyl phosphate (TXP) – A substance of very high concern (SVHC) because of its CMR<sup>\*</sup> properties Huiling Liu<sup>1</sup>, Håkon Midthaune<sup>1</sup>, Philip Ehlert<sup>2</sup> Jon Eigill Johansen<sup>1</sup>

<sup>1</sup>Chiron AS, Stiklestadveien 1, N-7041, Trondheim, Norway; <sup>2</sup> Institute for Chemistry and Material technology (NTNU), Høgskoleringen 5, N-7491, Trondheim, Norway

## **Introduction:**

Trixylyl phosphate (CAS 25155-23-1) is generally used as a flame retardant in hydraulic fluids and as a plasticizer. According to Regulation (EC) No. 1272/2008 (Annex VI, Part 3) trixylyl phosphate meets the criteria for classification as a reproductive toxin (Rep. 1B (H360F: "May damage fertility") in accordance with Article 57(c) of REACH (Regulation (EC) 1907/2006). Trixylyl phosphate (TXP) is a UVCB substance (substance of Unknown or Variable composition, Complex reaction produced of Unknown or Variable composition, Complex reaction, Comple through the reaction of phosphorus oxytrichloride and xylenols. The exact composition is unknown. In studies that form the basis for harmonized classification and labelling, the substance has been tested as such, but the individual constituents are not the basis for the classification. Nobile (1980) investigated the composition of two TXP products, and found the xylyl phosphate isomers 2,5-, 2,3-, 3,5-, 2,4- and 3,4- in decreasing order of abundance. The 2,6-isomer was not present. Other components identified included 4-ethylphenol, phenol, and trimethyl phenol. \*CMR: Carcinogenic, mutagenic, or toxic for reproduction.

## **Preparation of reference materials:**

Two samples of commercial TXP were tested and shown to have similar GC-MS and LC-UV chromatograms. The commercial trixylyl phosphate mixture was found to contain not only TXP, but a series of compounds with higher and lower molecular weights. The main task was to purify a sample containing the mass m/z 410 from the mixture. Focusing on the molecular weight distinction, the TXP mixture was successfully separated into five fractions, the one with the expected mass m/z 410, one with a higher mass containing one more methyl group, and three with lower masses, lacking 1-3 methyl group compared to that of TXP. The LC-UV chromatograms of the mixture and the separated fractions are shown in *Fig. 1a and 1b.* The GC-MS chromatogram of the technical mixture before separation is shown in *Fig. 2*. The GC-MS analysis and the mass spectra of the main peaks of each of the fractions are shown in *Fig. 3*.

## Synthesis of pure individual compounds and deuterated versions of TXP :

Chemical synthesis of pure individual compounds and deuterated versions of TXP and other organophosphate flame retardants are performed by reacting POCl<sub>3</sub> with pure xylenol or deuterated xylenol. Individual components of TXP, deuterated internal standard of TXP and many other organophosphates compounds are available as reference materials from Chiron.

Chiron No	Description	m/z
11143.24-100-IO	Tris(2,3-dimethylphenyl) phosphate	<i>m/z</i> 410
11144.24-100-IO	Trips(2,4-dimethylphenyl) phosphate	<i>m/z</i> 410
11145.24-100-IO	Tris(2,5-dmethylphenyl) phosphate	<i>m/z</i> 410
11146.24-100-IO	Tris(2,6-dimethylphenyl) phosphate	<i>m/z</i> 410
11147.24-100-IO	Tris(3,4-dimethylphenyl) phosphate	<i>m/z</i> 410
11148.24-100-IO	Tris(3,5-dimethylphenyl) phosphate	<i>m/z</i> 410





**11444.24-100-IO 2,4-TXP-d27 (Internal Standard)** 



Chiron No	Description	m/z	Abbreviation
11214.21-100-IO	Trixylylphosphate, purified Ion 368	<i>m/z</i> 368	TXP - 3xMethyl
11215.22-100-IO	Trixylylphosphate, purified Ion 382	<i>m/z</i> 382	TXP - 2xMethyl
1216.23-100-IO	Trixylylphosphate, purified Ion 396	<i>m/z</i> 396	TXP - 1xMethyl
10279.24-100-IO	Trixylylphosphate, purified Ion 410	<i>m/z</i> 410	TXP purified
11217.25-100-IO	Trixylylphosphate, purified Ion 424	<i>m/z</i> , 424	TXP + 1xMethyl



**Individual TXP components** are now available as reference materials from Chiron!