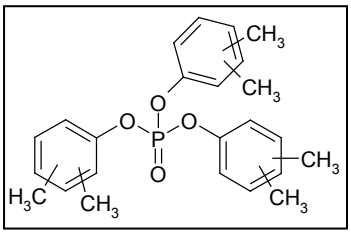
# Trixylyl phosphate (TXP)

## BMF 79 - Trixylyl phosphate (TXP)

### A SUBSTANCE OF VERY HIGH CONCERN (SVHC) BECAUSE OF ITS CMR* PROPERTIES




**Toxicity:**
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).

**Background:**
Trixylyl phosphate (TXP) is a UVCB substance (substance of Unknown or Variable composition, Complex reaction products, or Biological materials), thus contains over 50 different constituents. It has no additives and is produced through the reaction of phosphorus oxytrichloride and xylenols. The xylenols (dimethylphenols) are present in a distillation fraction of naturally occurring coal tar derivatives, which also contains different ethyl phenols. The reaction of the different xylenols and ethylphenols results in alkylated triphenyl phosphates with a high amount of possible isomers that cannot be easily analysed according to ECHA (European chemical agency).

Therefore, 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)[1] 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, p-cresol, 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.*

**Available standards:**
These individual TXP components are now available as reference materials from Chiron.**

| Chiron No. | Description | *m/z* | Abbreviation |
|---|---|---|---|
| **Separated fraction:** | | | |
| 11214.21-100-IO * | Trixylylphosphate, purified Ion *m/z* 368 (trimethyl) | *m/z* 368 | TXP-3xMethyl |
| 11215.22-100-IO | Trixylylphosphate, purified Ion *m/z* 382 (tetramethyl) | *m/z* 382 | TXP-2xMethyl |
| 11216.23-100-IO | Trixylylphosphate, purified Ion *m/z* 396 (pentamethyl) | *m/z* 396 | TXP-1xMethyl |
| **10279.24-100-IO** | **Trixylylphosphate, purified Ion *m/z* 410 (hexamethyl)** | ***m/z* 410** | **TXP purified** |
| 11217.25-100-IO | Trixylylphosphate, purified Ion *m/z* 424 (heptamethyl) | *m/z* 424 | TXP+1xMethyl |
| | | | |
| **Technical mixture:** | | | |
| 10265.24-100-IO | Trixylylphosphate, technical mixture | | TXP |
| 10265.24-K-IO | Trixylylphosphate, technical mixture | | TXP |
| 10265.24-50MG | Trixylylphosphate, technical mixture | | TXP |
| | | | |
| **Individual compounds:** | | | |
| 2135.21-100-IO | Tris(2-methylphenyl) phosphate (ortho) | *m/z* 368 | 2-TTP |
| 2134.21-100-IO | Tris(3-methylphenyl) phosphate (meta) | *m/z* 368 | 3-TTP |
| 2136.21-100-IO | Tris(4-methylphenyl) phosphate (para) | *m/z* 368 | 4-TTP |
| 2137.21-100-IO | Tris(methylphenyl) phoshate, mix of isomers | *m/z 368* | TTP |
| 11143.24-100-IO | Tris(2,3-dimethylphenyl) phosphate | *m/z* 410 | 2,3-TXP |
| 11144.24-100-IO | Tris(2,4-dimethylphenyl) phosphate | *m/z* 410 | 2,4-TXP |
| 11145.24-100-IO | Tris(2,5-dmethylphenyl) phosphate | *m/z* 410 | 2,5-TXP |
| 11146.24-100-IO | Tris(2,6-dimethylphenyl) phosphate | *m/z* 410 | 2,6-TXP |
| 11147.24-100-IO | Tris(3,4-dimethylphenyl) phosphate | *m/z* 410 | 3,4-TXP |
| 11148.24-100-IO | Tris(3,5-dimethylphenyl) phosphate | *m/z* 410 | 3,5-TXP |

Ref: (1) http://echa.europa.eu/documents/10162/19377756/supdoc_trixylyl_phosphate_en.pdf
*100-IO = 100µg/mL in isooctane, K-IO = 1000µg/mL in isooctane
**For products, pack sizes and presentations not listed, please contact sales@chiron.no

*Figure 1a:* LC-UV chromatogram of technical trixylyl phosphate

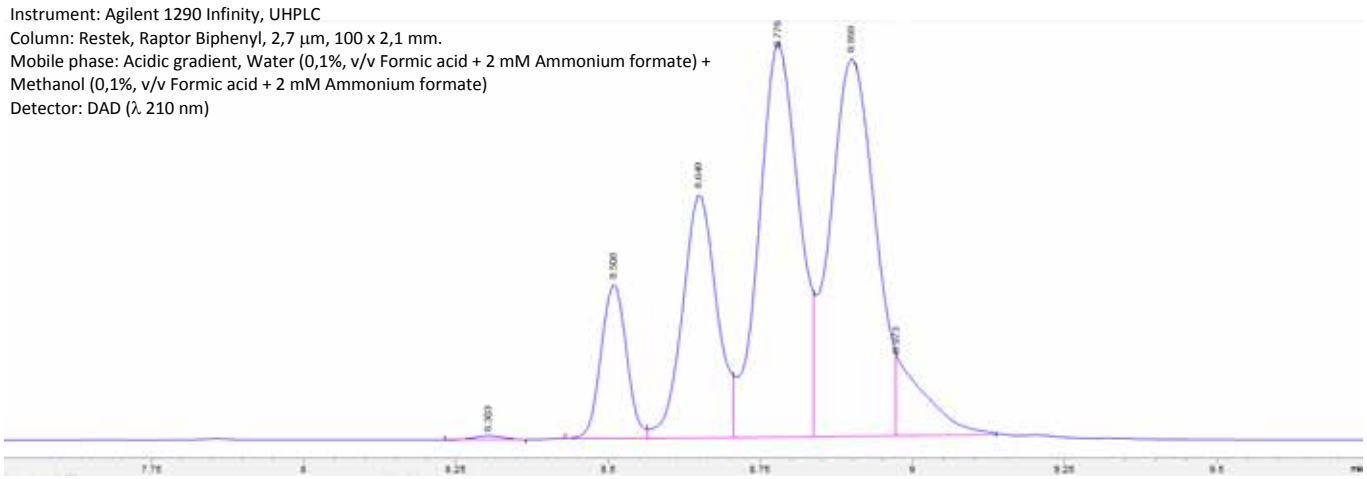



*Figure 1b:* LC-UV after separation of 5 fractions of the technical trixylyl phosphate

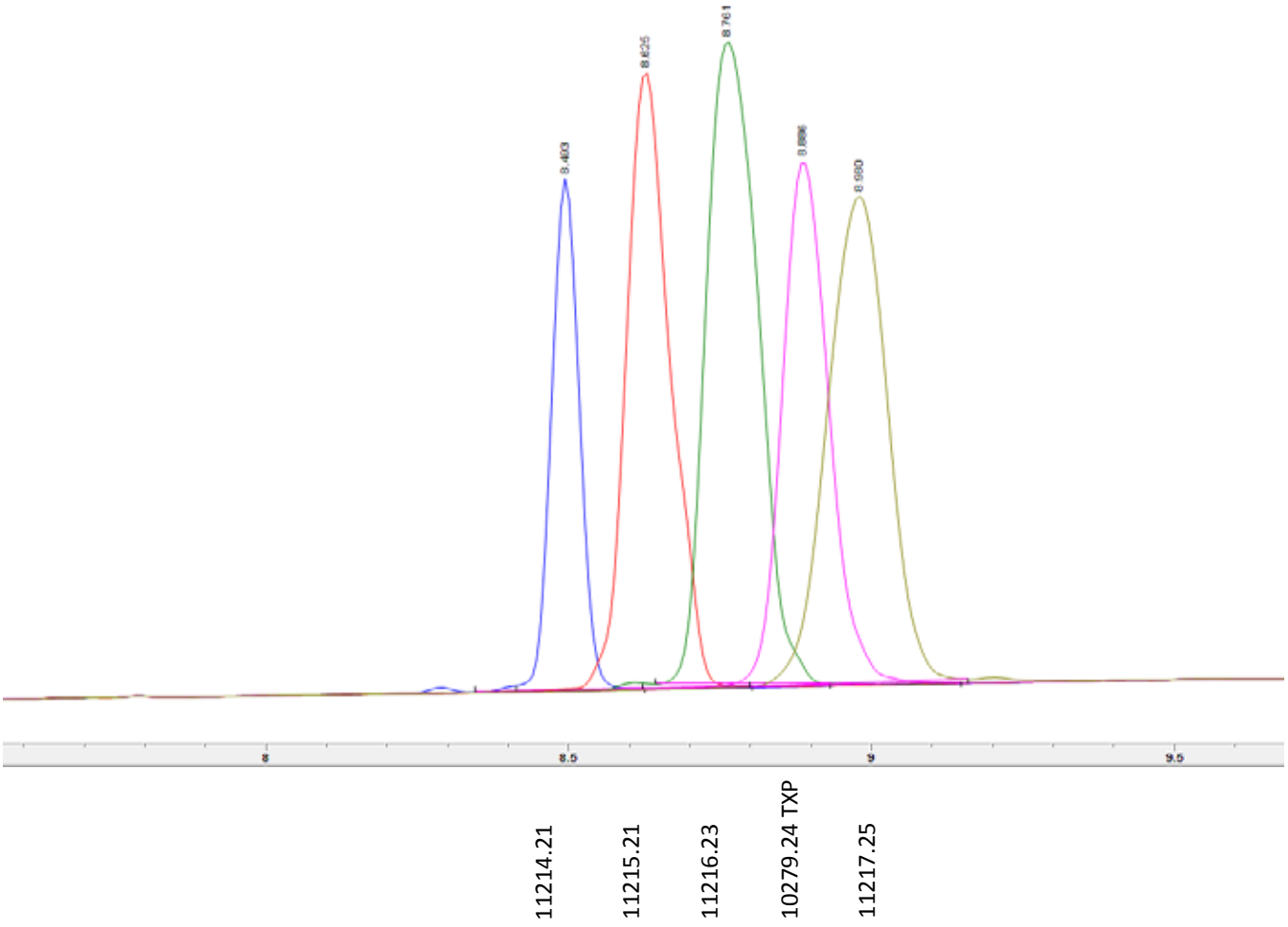


*Figure 2:* GC-MS of technical trixylyl phosphate

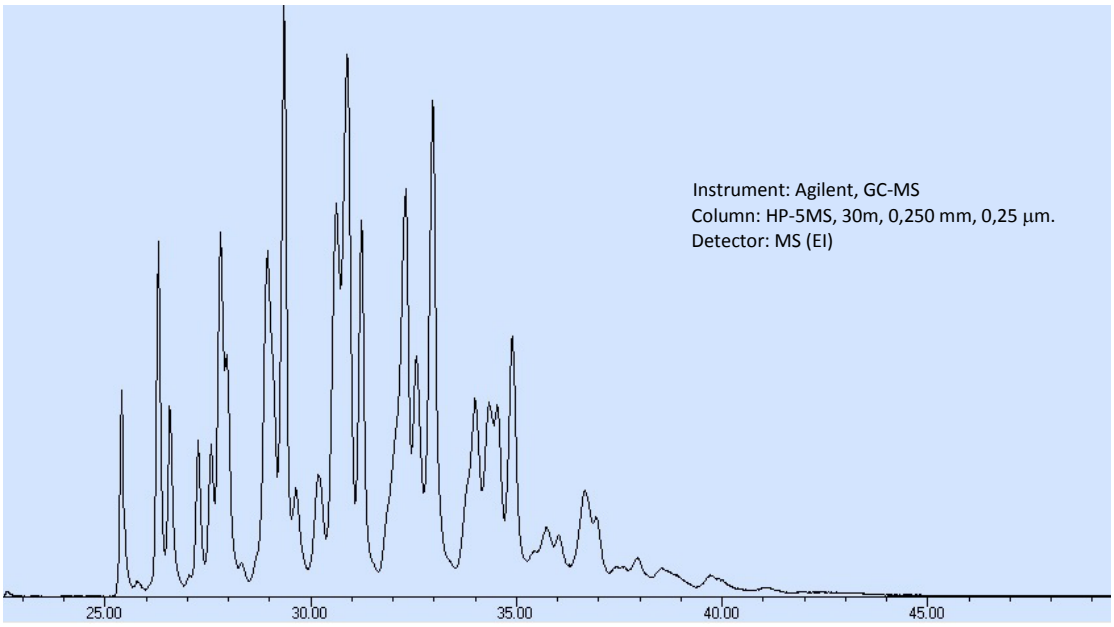
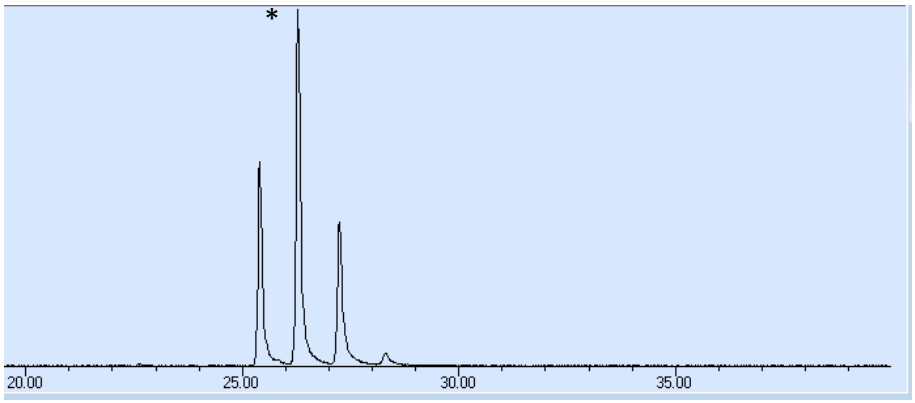
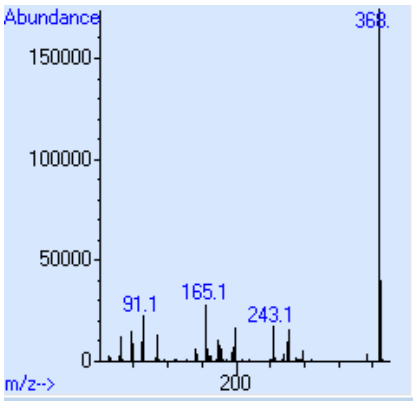


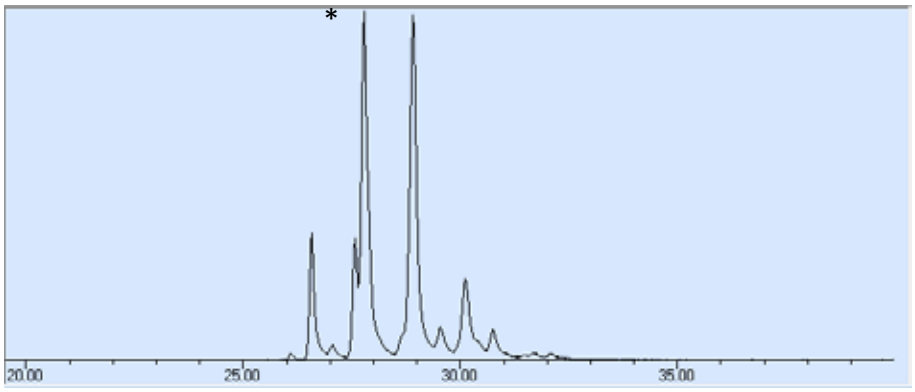

*Figure 3:* GC-chromatograms and mass spectra of 5 trixylyl phosphate fractions (of peak *)

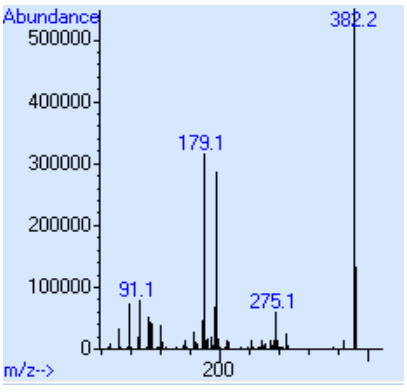
11214.21
TXP-3xMethyl (m/z 368)



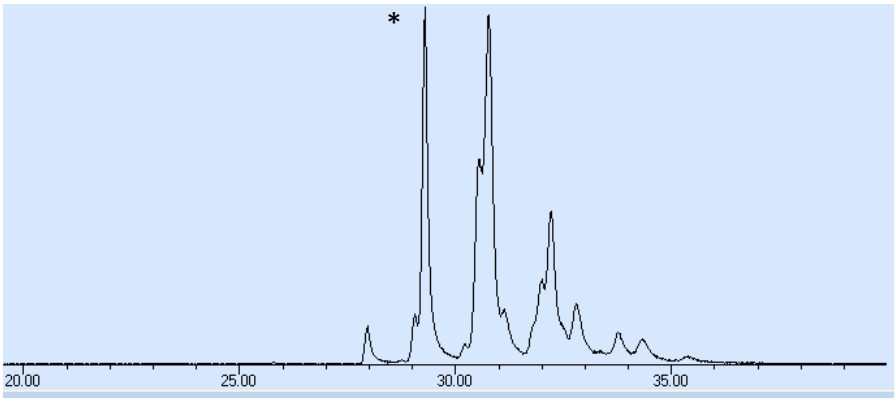



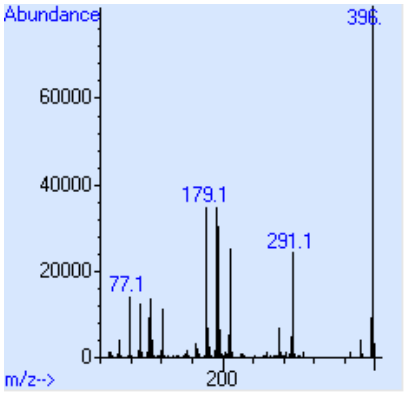

11215.22
TXP-2xMethyl (m/z 382)



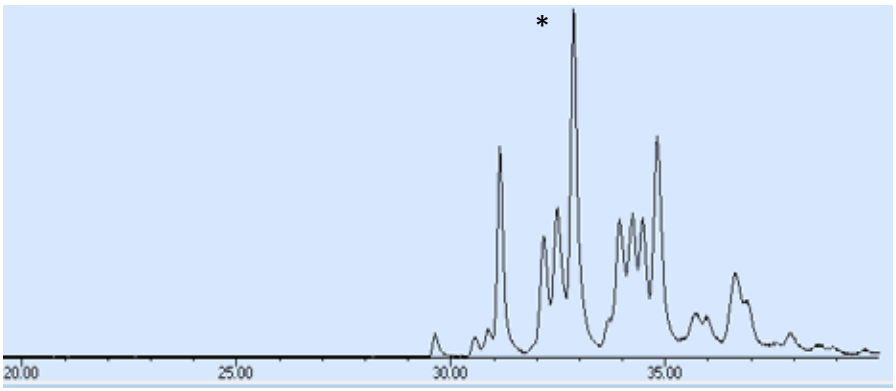



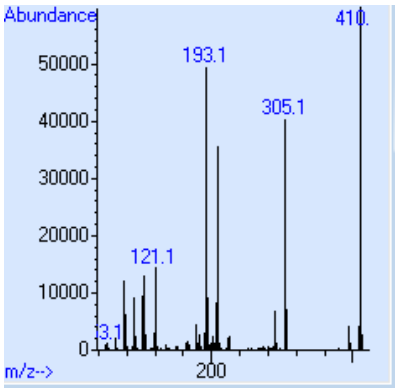
11216.23
TXP-1xMethyl (m/z 398)



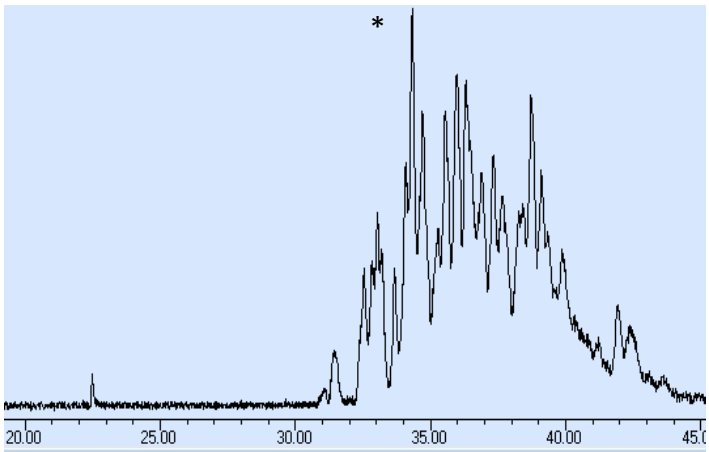



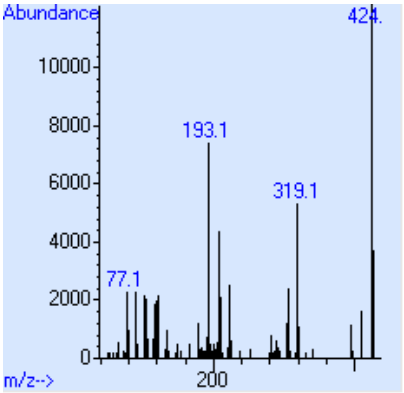

10279.24
TXP purified (m/z 410)




11217.25
TXP+1 xMethyl (m/z 428)



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