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An overview of the environmental risk evaluation reports for aryl phosphate esters

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Steve Killeen

**Head of Science** 

Steve Killeen

# Introduction

This series of reports evaluates a group of related substances that represent the major aryl phosphate ester products used in Europe:

Triphenyl phosphate
Trixylenyl phosphate
Tricresyl phosphate
Cresyl diphenyl phosphate
Tris(isopropylphenyl) phosphate
Isopropylphenyl diphenyl phosphate
Tertbutylphenyl diphenyl phosphate
2-Ethylhexyl diphenyl phosphate
Isodecyl diphenyl phosphate
Tetraphenyl resorcinol diphosphate

A further substance is known to be commercially available, but it has already been assessed under the Notification of New Substances (NONS) Regulations. Information is also available on some (possibly obsolete) triaryl phosphates that are not thought to be supplied in the EU. This information is summarised in Annex A, but the risks from these products have not been assessed. Information for the group as a whole has also been used in this assessment, where appropriate, to fill any gaps in the database for this particular substance. Annex B discusses the read-across of data between the various phosphate esters considered.

This group was highlighted for assessment during preliminary work for an Environment Agency review of flame retardants, particularly because they are potential replacements for other flame retardants that have already been identified as a risk to health or the environment. Regulators need to understand the potential consequences of such market switches before substantial replacement takes place. These assessments are not intended to provide a basis for comparison between the different aryl phosphates themselves; such a comparison would require consideration of a wider range of factors than are included here (such as human health risks, efficacy, recycling potential and costs). The assessments have been produced as part of the UK Coordinated Chemical Risk Management Programme (UKCCRMP) (http://www.defra.gov.uk/environment/chemicals/ukrisk.htm).

The methodology used in the report follows that given in an EU Technical Guidance Document (TGD)¹ for risk assessment of existing substances. The scientific work was mainly carried out by the Building Research Establishment Ltd (BRE), under contract to the Environment Agency. The review of mammalian toxicity data for the assessment of non-compartment specific effects was carried out by the Institute of Environment and Health, under contract to the Department for Environment, Food and Rural Affairs (Defra).

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<sup>&</sup>lt;sup>1</sup> This document has recently been replaced by similar guidance for the REACH Regulation.

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# 1 General substance information

The identity and physico-chemical properties of the aryl phosphate esters considered in the risk assessments are shown in Table 1.1. A summary of the names, tradenames, abbreviations and registered trademarks of aryl phosphate esters is given in Table 1.2.

Most of the commercial aryl phosphate esters are complex isomeric mixtures and the actual composition will vary between different commercial products and manufacturers. They have generally been assumed to behave as single substances in the environment for the purposes of these assessments, because there is currently no practical way of dealing with this complexity in any other way.

Additives are not thought to be present in the commercially supplied products, although some may be supplied as blends with other (halogenated) flame retardants.

The purity and composition of the main groups of aryl phosphate products considered in the assessment are discussed below.

- Triphenyl phosphate is produced with a purity above 99.6 per cent.
- The commercial cresyl diphenyl phosphate products are supplied as mixtures containing isomers (mainly meta- and para-) of cresyl diphenyl phosphate, along with triphenyl phosphate (25 per cent), dicresyl phenyl phosphate and tricresyl phosphate (5.5 per cent). The level of orthocresyl isomers in the products currently supplied is under 0.02 per cent.
- Tricresyl phosphate is supplied as a relatively pure mixture of *meta-* and *para-* isomers. The amount of *ortho-* isomers present is minimized owing to their toxicity. A small amount of triphenyl phosphate (0.5 per cent) may also be present.
- Trixylenyl phosphate is supplied as an isomeric mixture based on the 2,5-, 2,3-, 3,5-, 2,4- and 3,4-xylenol isomers.
- The commercially supplied isopropylated phenyl phosphates cover a spectrum of products ranging from isopropylphenyl diphenyl phosphate to tris(isopropylphenyl) phosphate. These are isomeric mixtures of phosphate esters based on phenol and isopropyl phenol, and the various products also contain differing amounts of triphenyl phosphate (ranging from 4 to 35 per cent depending on the product).
- For tertbutylphenyl diphenyl phosphate, the isomer distribution and the
  distribution of alkylation levels may vary between products from different
  manufacturers. One product was reported to contain 15-20 per cent
  triphenyl phosphate with the remainder primarily consisting of isomers of
  tertbutylphenyl diphenyl phosphate, along with di-tertbutylphenyl
  diphenyl phosphate.
- 2-Ethylhexyl diphenyl phosphate is supplied as a 94.5 per cent pure substance, with a triphenyl phosphate content of below 4 per cent.
- The commercially supplied isodecyl diphenyl phosphate is reported to contain over 90 per cent isodecyl diphenyl phosphate and under 5 per cent triphenyl phosphate. Other components present may include di-isodecyl phenyl phosphate.

Table 1.1 Identity and physico-chemical properties of aryl phosphate esters

Property					Subst	tance				
Name	Triphenyl phosphate	Cresyl diphenyl phosphate	Tricresyl phosphate	Trixylenyl phosphate	Isopropyl phenyl diphenyl phosphate	Tris(isoprop -ylphenyl) phosphate	Tertbutyl phenyl diphenyl phosphate	2- Ethylhexyl diphenyl phosphate	Isodecyl diphenyl phosphate	Tetraphenyl resorcinol diphosphate
CAS No.	115-86-6	26444-49-5	1330-78-5	25155-23-1	28108-99-8	26967-76-0 68937-41-7	56803-37- 3 68937-40- 6	1241-94-7	29761-21-5	57583-54-7
EINECS No.	204-112-2	247-693-8	215-548-8	246-677-8	248-848-2	248-147-1 273-066-3	260-391-0 273-065-8	214-987-2	249-828-6	260-830-6
Molecular weight g/mol	326.29	340.32	368.37	410.45	368.37	452.54	382.40	362.4	390.5	574.47
Melting point °C	49	-35	-30	-20	-26	-26	-21	-60	<-50	<20
Boiling point (at atmospheric pressure) °C	370-500	390	>300	>300	>300	>300	420	375	>245	>300
Vapour pressure Pa at 20°C	1.2×10 <sup>-3</sup>	3.3×10 <sup>-5</sup>	3.5×10 <sup>-5</sup>	8.7×10 <sup>-6</sup>	9.5×10 <sup>-6</sup>	2.6×10 <sup>-6</sup>	7.8×10 <sup>-5</sup>	3.4×10 <sup>-4</sup>	3.6×10 <sup>-5</sup>	8.7×10 <sup>-6</sup>
Water solubility mg/l at room temperature	1.9	2.6	0.36	0.89	2.2 mg/l at 20°C	0.12 mg/l at 20°C	0.04-3.2	0.0506	0.011	0.69
Log K <sub>ow</sub>	4.63	4.51	5.11	5.63	5.3	6.1	5.12	5.73	5.44	5.5
Henry's law constant Pa m³/mol at 20°C	0.21	0.0043	0.036	0.0040	0.0016	0.0087	0.009	4.44 Pa m³/mol at 25°C	1.8 Pa m³/mol at 25°C	0.0072

Note: for details of the composition of the products tested or the structures used to obtain these values, please see the individual assessment reports.

• Tetraphenyl resorcinol diphosphate contains a maximum of 5 per cent triphenyl phosphate (typically 1 to 2 per cent) and a maximum of 0.05 per cent free phenol. Production of the substance also leads to the production of oligomers which contain additional resorcinol phenylphosphate groups in the chain. Hence triphosphate, tetraphosphate and higher oligomers may be present. One commercial substance contained 68 per cent tetraphenyl resorcinol diphosphate; 19 per cent triphosphate; 6 per cent tetraphosphate; 3 per cent higher oligomers; and 4 per cent triphenyl phosphate.

Table 1.2 Summary of other names, abbreviations, tradenames and registered trademarks of aryl phosphate esters

Abbreviations, tradenames and registered trademarks
Celluflex 179C®, Disflamoll TKP®, Kolflex 5050®, Kronitex R®, Kronitex TCP®, Phosflex 179®, Phosflex Lindol®, Pliabrac 521®, Pliabrac TCP®, Phosphoric acid, tricresyl ester, Phosphoric acid, tris(methylphenyl) ester, Phosphoric acid, tritolyl ester, PX-917®, Santicizer 140®, TCP, Tricresol phosphate and Tritolyl phosphate.
Antiblaze TXP®, Fyrquel 220® (historic only; the modern product is no longer based on trixylenyl phosphate), Fyrquel EHC®, Kronitex TXP®, Phosflex 179A®, Phosphoric acid, trixylyl ester, Pliabrac TXP®, Reolube TXP®, Tris(dimethylphenyl) phosphate, Trixylyl phosphate, TXP and Xylenol, phosphate ester.
Durad 220B <sup>®</sup> , Fyrquel GT <sup>®</sup> , Phosflex 71B <sup>®</sup> , Santicizer 154 <sup>®</sup> , TB220-H <sup>®</sup> , TB220-L <sup>®</sup> and TBDPP.
Durad 300°, DURAD 310M°, Isopropylated phenyl phosphate, Kronitex 50°, Kronitex 100°, Kronitex 200°, Phosflex 31 P°, Reofos 35°, Reofos 50°, Reofos 65°, Reofos 95°, Reofos 120°, Reolube HYD 46° and Triaryl phosphates isopropylated.
EHDP, Diphenyl 2-ethylhexyl phosphate, Disflamoll DPO®, Phosflex 362®, Phosphoric acid, 2-ethylhexyl diphenyl ester and Santicizer 141®.
IDDP, Phosflex 390 <sup>®</sup> and Santicizer 148 <sup>®</sup> .
Fyrolflex RDP®, Phosphoryl chloride, polymer with 1,3-benzenediol phenyl ester, RDP, Reofos RDP®, Resorcinol bis(diphenyl phosphate.
Celluflex TPP <sup>®</sup> , Disflamoll TP <sup>®</sup> , Phosflex TPP <sup>®</sup> , Phosphoric acid, triphenyl ester, Pilabrac 521 <sup>®</sup> , Reofos TPP <sup>®</sup> , Reomol TPP <sup>®</sup> and TPP.
CDP, Diphenyl cresyl phosphate, Diphenyl tolyl phosphate, Methylphenyl diphenyl phosphate, Monocresyl diphenyl phosphate Phosphoric acid, diphenyl tolyl ester, Phosphoric acid, cresyl diphenyl ester, Phosphoric acid, methylphenyl diphenyl ester, Tolyl diphenyl phosphate, Disflamoll® DPK, Kronitex® CDP, Phosflex® CDP and Santicizer® 140.

Some of the tradenames and trademarks may refer to older products no longer supplied to the EU, or products produced outside the EU, but these are included in the report as they are sometimes referred to in the open literature.

# 2 Uses

The main uses of the main commercial aryl phosphate products supplied in the EU are summarised in Table 2.1. Aryl phosphates are generally used as flame-retardant additives in polymer systems but some are also used as fire-resistant hydraulic fluids, lubricants and lubricant additives.

Table 2.1 Main uses of aryl phosphate products supplied in the EU

Product							,	Use						
_	Textile coating	Adhesives	Paints	Pigment dispersions	Printed circuit boards	PVC	Polyurethane	Thermoset resins	Thermoplastic / stryrenic resins	Rubber	Photographic film	<b>Lubricant</b> additive	Hydraulic fluid	Power generation fluid
Triphenyl phosphate					×			×	×		×			
Cresyl diphenyl phosphate	×	×				×	×	×	×			×		
Tricresyl phosphate		×		×		×	×				×	×		
Trixylenyl phosphate														×
Tertbutylphenyl diphenyl phosphate	×					×	×					×	×	×
Isopropylated phenyl phosphates <sup>a</sup>	×	×	×	×		×	×		×			×	×	×
2-Ethylhexyl diphenyl phosphate	×	×	×	×		×	×			×	×			
Isodecyl diphenyl phosphate	×		×	×		×	×			×				
Tetraphenyl resorcinol diphosphate			×	×		×	×		×					

Notes:

a) This covers both isopropylphenyl diphenyl phosphate and tris(isopropylphenyl) phosphate.

# 3 Environment

# 3.1 Exposure

The most relevant characteristics of aryl phosphate esters are summarised in Table 1.1 (physico-chemical properties) and Table 3.1 (environmental fate data). Table 3.2 shows the measured data and some predicted values used in Annex B to estimate missing data. In very general terms, aryl phosphates:

- Are readily or inherently biodegradable.
- May hydrolyse, particularly at high or low pHs.
- Have atmospheric half-lives of 8 to 36 hours.
- Have low water solubilities and vapour pressures.
- Have relatively high log  $K_{ow}$  values and hence organic carbon water partition coefficients ( $K_{oc}$  2,400-14,400 l/kg).
- Have moderate bioconcentration factors (BCF) in fish (200-1,990 l/kg).

The relatively high log  $K_{ow}$  values indicate that aryl phosphate esters will adsorb strongly onto sludge and sediment and would not be expected to be mobile in soil. The potential for uptake and accumulation of the substances by fish and other aquatic organisms appears to be moderate.

The predicted fate of aryl phosphate esters in waste water treatment plant depends on the actual biodegradability of each substance, but adsorption onto sewage sludge is expected to occur. Therefore, emissions to waste water from industry may end up in both surface water and soil via spreading of sewage sludge onto agricultural land. Although aryl phosphate esters generally have low vapour pressures, emissions to air could still occur from some sources, particularly where elevated temperatures are involved (such as during polymer processing) or when extended time periods are considered (such as emissions over lifetime of polymer products containing aryl phosphates). Similarly, leaching from articles could occur over extended time periods if the articles came into regular contact with water.

Emissions of aryl phosphates were estimated over their whole lifecycle using information relevant to the various industries considered in conjunction with the default emission factors from a European Technical Guidance Document (TGD). In most cases, information on the industries comes from Emission Scenario Documents (ESD) or from assessments of other substances. Producers of the aryl phosphates provided information on the amounts used by representative large customers, and this was used in the local estimates of emissions from use. Some additional information was provided for some substances on waste treatment and cleaning at a small number of user sites; this information did not contradict the assumptions made on the basis of the ESDs. These aspects are considered further in Section 4.1. The total EU estimated emissions are summarised in Table 3.3.

Methods described in the TGD were used to estimate predicted environmental concentrations (PECs) for each aryl phosphate ester product considered for water, sediment, sewage treatment plants, air, soil and biota. Table 3.4 shows the range of PEC values calculated for the various stages of the lifecycle for each substance. The calculated concentrations in air are very low and so are not included here. Insufficient measured data are available to make any judgment on the validity of PECs for the local emission scenarios.

 Table 3.1
 Summary of environmental behaviour of aryl phosphate esters

Substance				Prop	perty				
riphenyl phosphate  Cresyl diphenyl phosphate  ricresyl phosphate  rixylenyl phosphate  ertbutylphenyl liphenyl phosphate sopropylphenyl liphenyl phosphate  ris(isopropyl- phenyl) phosphate	Bio- degradability	Atmospheric half-life	Hydrolysis half-life	Pre		haviour in w atment plant		Organic carbon-water	Bio- concentration
		(hours)		% degraded	% adsorbed to sludge	% volatilized to air	% to effluent	partition coefficient (K <sub>oc</sub> ) (I/kg)	factor for fish (BCF) (I/kg)
Triphenyl phosphate	Readily biodegradable	36	3 days at pH 9 19 days at pH 7 >28 days at pH 5	50.6	41.0	0.09	8.27	10,000	420
Cresyl diphenyl phosphate	Readily biodegradable	32.1	No data	54.4	18.5	5.2×10 <sup>-3</sup>	27.0	2,398	200
Tricresyl phosphate	Readily biodegradable	27.5	30-40 days at pH 8 1,100-2,200 years at pH 7	62.8	27.5	0.020	9.64	4,720	800
Trixylenyl phosphate	Inherently biodegradable	8.2	30-40 days at pH 8 1,100 years at pH 7	0	49.4	3.7×10 <sup>-3</sup>	50.6	8,486	1,900
Tertbutylphenyl diphenyl phosphate	Readily biodegradable	24.1	32-45 days at pH 8 1,100 years at pH 7	46.4	29.9	0.01	23.7	4,773	778
Isopropylphenyl diphenyl phosphate	Readily biodegradable	21.4	39 days at pH 8 1,100 years at pH 7	43.7	33.8	1.58×10 <sup>-3</sup>	22.5	5,848	564
Tris(isopropyl- phenyl) phosphate	Inherently biodegradable	11.7	39 days at pH 8 1,100 years at pH 7	16.3	56.1	4.3×10 <sup>-3</sup>	27.5	14,421	1,986
2-Ethylhexyl diphenyl phosphate	Readily biodegradable	9.7	No data	36.1	43.3	1.63	19.0	9,499	934
Isodecyl diphenyl phosphate	Inherently biodegradable	9.2	No data	23.1	40.1	1.2	35.6	6,849	335

Substance				Prop	perty				
	Bio- degradability	Atmospheric half-life	Hydrolysis half-life	Pre		aviour in w tment plan		Organic carbon-water	Bio- concentration
		(hours)		% degraded	% adsorbed to sludge	% volatilized to air	% to effluent	partition coefficient (K <sub>oc</sub> ) (I/kg)	factor for fish (BCF) (I/kg)
Tetraphenyl resorcinol diphosphate	Inherently biodegradable	18.3	21 days at pH 9 17 days at pH 7 11 days at pH 4	0	46.0	0.01	54.0	7,328	969

Table 3.2 Data used for estimating missing values

Phosphate ester				Pro	perty				
	Measured vapour	Measured water solubility	Measured log K <sub>ow</sub>	Measured BCF (I/kg)	•	term NOEC for a organisms (mg/l)	•	EPI estima	ates
	pressure at 20°C (Pa)	at room temperature (mg/l)			Fish	Invertebrates	Algae	Vapour pressure at 25°C (Pa)	Log K <sub>ow</sub>
Triphenyl phosphate	1.2×10 <sup>-3</sup>	1.9	4.63	420	0.037		0.1	2.8×10 <sup>-5</sup>	4.70
Trixylenyl phosphate	[4.7×10 <sup>-4</sup> ] <sup>a</sup>	0.89	5.63	1,300- 1,900				2.7×10 <sup>-6</sup>	7.98
Tricresyl phosphate	3.5×10 <sup>-5</sup>	0.36	5.11	800	0.00032	0.1	0.32	3.4×10 <sup>-6</sup>	6.34
Cresyl diphenyl phosphate	3.3×10 <sup>-5</sup>	2.6	4.51	200				1.4×10 <sup>-5</sup>	5.24
Tris(isopropylphenyl) phosphate	2.3×10 <sup>-6</sup>				0.024 <sup>b</sup>	0.006 <sup>b</sup>		2.7×10 <sup>-6</sup>	9.07
Isopropylphenyl diphenyl phosphate	9.5×10 <sup>-6</sup>	2.2	5.30	[7,266] <sup>a</sup>	0.024 <sup>b</sup>	0.006 <sup>b</sup>		5.3×10 <sup>-6</sup>	6.16
Tertbutylphenyl diphenyl phosphate	7.8×10 <sup>-5</sup>	0.04-3.2	5.12	778	0.093	0.010		3.5×10 <sup>-6</sup>	6.61
2-Ethylhexyl diphenyl phosphate	3.4×10 <sup>-4</sup>	0.38-1.9 <sup>c</sup>	5.73	934	0.021	0.018		2.5×10 <sup>-5</sup>	6.30
Isodecyl diphenyl phosphate	[3.8] <sup>a</sup>	0.03-0.75 <sup>c</sup>	5.44	335	0.057	0.004		6.3×10 <sup>-6</sup>	7.28
Tetraphenyl resorcinol diphosphate		0.69				>0.064		2.7×10 <sup>-6</sup>	7.41

Notes:

a) These values are uncertain (see main risk assessment reports) and have not been included in the estimation analysis.b) Assumes these two products have similar toxicity.c) Revised solubilities used in the individual risk assessment reports, the values here are used in the estimation analysis.

Table 3.3 Total estimated emissions in the EU

Product	Media							Total	estimated	d emissic	ns in the l	EU (kg/	year)					
		Production	Textile coating	Adhesives	Paints	Pigment dispersions	Printed circuit boards	PVC	Polyurethane	Thermoset resins	Thermoplastic/ stryrenic resins	Rubber	Photographic film	Lubricant additive	Hydraulic fluid	Power generation fluid	Miscellaneous	Total
Triphenyl	Air						11			212	673		5,775				20	6,691
phosphate	Water	352					78			885	8,063		567				30	9,975
	Soil						145			1,034	15,725						50	16,954
Cresyl	Air		19	21				10,078	677	84	<1			<<1			2,440	13,319
diphenyl	Water	503	359	14,932				34,488	5,647	1,431	10			552			12,870	70,792
phosphate	Soil		691	964				19,645	16,412	2,122	30			544			9,050	49,458
Tricresyl	Air			2		2		6,288	50				159	140,054			1,489	148,044
phosphate	Water	86		633		252		2,497	474				24	<1			889	4,855
	Soil			80		750		4,601	1,400								1,565	8,396
Trixylenyl	Air															4		4
phosphate	Water	1,040														<1		1,040
	Soil																	
Tertbutyl	Air		15					583	316					<<1	<<1	<1		914
phenyl	Water	56	288					4,132	2,640					3,257	980	<<1		11,353
diphenyl phosphate	Soil		564					1,896	7,646					3,210	3,920			17,236
Isopropyl	Air		88	neg.	4,300	<1		1,576	153		<<1			<1	<<1		154	6,271
phenyl	Water	1,811	6,982	neg.	45,154	88		186,934	5,649		5			4,760	480		15,025	266,888
diphenyl phosphate	Soil		13,810	neg.	25,820	265		55,186	16,620		15			19,040	1,920		9,273	141,949

Table 3.3 continued.

Product	Media							Total est	imated em	issions	s in the El	J (kg/ye	ar)					
		Production	Textile coating	Adhesives	Paints	Pigment dispersions	Printed circuit boards	PVC	Polyurethane	Thermoset resins	Thermoplastic/ stryrenic resins	Rubber	Photographic film	Lubricant additive	Hydraulic fluid	Power generation fluid	Miscellaneous	Total
Tris	Air		26	2	10	5		87	4					<<1	1	neg.	10	145
(isopropyl	Water	760	1,712	3,799	323	1,160		6,567	158					3,040	696	neg.	1,334	19,549
phenyl) phosphate	Soil		4,063	480	290	3,450		3,815	465					12,150	1,624	neg.	2,013	28,350
2-	Air		997	228	32,276	9		64,563	196			152	795				4,627	103,843
Ethylhexyl	Water	13,572	4,398	18,994	12,915	384		48,195	362			527	58				4,037	103,442
diphenyl phosphate	Soil		7,781	2,400	11,670	1,130		63,254	971			745					4,102	92,053
Isodecyl	Air		19		868	2		5,871	59			31					45	6,895
diphenyl	Water	9,000	247		1,549	252		23,340	492			284					169	35,333
phosphate	Soil		690		2,938	750		54,696	1,430			750					395	61,649
Tetra	Air				6	1		1	28		160						<1	196
phenyl	Water	1,547			81	151		166	1,018		18,170						36	21,169
resorcinol di phosphate	Soil				75	450		65	3,010		53,490						106	57,196

Notes:

Neg. = losses from these areas cannot be quantified but are thought to be negligible.

Table 3.4 Predicted environmental concentrations

	Media									PEC							
Product		Production	Textile coating	Adhesives	Paints	Pigment dispersions	Printed circuit boards	PVC	Polyurethane	Thermoset resins	Thermoplastic/ stryrenic resins	Rubber	Photographic film	Lubricant additive	Hydraulic fluid	Power generation fluid	Regional sources
	Water (µg/I)	0.03 - 0.3					0.52 - 5.51			0.52 – 5.51	1.48 – 15.9		0.52 – 5.51	-			0.011
	Sediment (mg/kg wet weight)	6.3×10 <sup>-3</sup> - 0.07					0.11 – 1.2			0.11 – 1.2	0.32 – 3.48		0.11 – 1.2				2.4×10 <sup>-3</sup>
Triphe	WWTP (mg/l)	0.01– 1.0					5.2×10 <sup>-3</sup> – 0.06			$5.2 \times 10^{-3} - 0.06$	0.01 – 0.16		5.2×10 <sup>-3</sup> – 0.06				
Triphenyl phosphate	Soil (mg/kg wet weight)	neg.					0.16 – 1.74			0.16 – 1.74	0.47 – 5.04		0.16 – 1.74				7.7×10 <sup>-5</sup> – 5.1×10 <sup>-3</sup>
sphate	Secondary poisoning – fish (mg/kg)	7.6×10 <sup>-3</sup> – 0.06					0.02 – 0.15			7.4×10 <sup>-3</sup> – 0.95	0.26 – 2.76		0.09 – 0.95				0.1 10
	Secondary poisoning – earthworm (mg/kg)	neg.			<u>.</u>		0.19 – 2.0			0.19 – 2.0	0.53 – 5.78		0.19 – 2.0				

Table 3.4 continued.

	Media								PEC								
Product		Production	Textile coating	Adhesives	Paints	Pigment dispersions	Printed circuit boards	PVC	Polyurethane	Thermoset resins	Thermoplastic/ stryrenic resins	Rubber	Photographic film	Lubricant additive	Hydraulic fluid	Power generation fluid	Regional sources
	Water (µg/l)	0.13 – 0.41	0.78 – 1.05	neg.				0.28 – 4.42	1.32 – 4.82	0.45 – 1.45	0.24 - 0.65			0.12			0.11
C	Sediment (mg/kg wet weight)	6.72×10 <sup>-3</sup> – 0.02	0.02 – 0.06	neg.				0.01 – 0.23	0.07 – 0.26	0.02 – 0.08	0.01 – 0.03			6.53×10 <sup>-3</sup>			3.1×10 <sup>-3</sup>
resylo	WWTP (mg/l)	0.01 – 1.0	2.7×10 <sup>-3</sup> – 9.46×10 <sup>-3</sup>	neg.				1.69×10 <sup>-3</sup> – 0.04	0.01 – 0.05	3.4×10 <sup>-3</sup> – 0.01	1.35×10 <sup>-3</sup> – 5.4×10 <sup>-3</sup>			1.47×10 <sup>-4</sup>			
Cresyl diphenyl	Soil (mg/kg wet weight)	neg.	6.58×10 <sup>-3</sup> – 0.02	neg.				4.13×10 <sup>-3</sup> – 0.11	0.03 – 0.12	8.24×10 <sup>-3</sup> – 0.03	3.34×10 <sup>-3</sup> – 0.01			3.96×10 <sup>-4</sup>			3.4×10 <sup>-5</sup> - 5.0×10 <sup>-3</sup>
phosphate	Secondary poisoning – fish (mg/kg)	0.02 – 0.05	0.02 – 0.03	neg.				0.02 – 0.38	0.12 – 0.41	0.03 – 0.06	0.02 – 0.07			0.02			
ate	Secondary poisoning – earthworm (mg/kg)	neg.	0.02 – 0.06	neg.				0.01 – 0.27	0.08 – 0.29	0.02 – 0.08	8.66×10 <sup>-3</sup> – 0.03			1.21×10 <sup>-3</sup>			

Table 3.4 continued.

	Media							PEC								
Product		Production	Textile coating	Adhesives	dispersions Paints	boards	PVC	Polyurethane	Thermoset resins	Thermoplastic/ stryrenic resins	Rubber	Photographic film	Lubricant additive	Hydraulic fluid	Power generation fluid	Regional sources
	Water (µg/l)	0.02 – 0.1		neg.	0.3	37	0.01 -0.63	0.03 - 0.29				0.03 – 0.29	7.34×10 <sup>-3</sup>			5.8×10 <sup>-3</sup>
	Sediment (mg/kg wet weight)	2.5x10 <sup>-3</sup> – 0.01		neg.	0.0	)4	1.1×10 <sup>-3</sup> – 0.06	3.1×10 <sup>-3</sup> – 0.03				3.1×10 <sup>-3</sup> – 0.03	7.59×10 <sup>-4</sup>			6.1×10 <sup>-4</sup>
Tric	WWTP (mg/l)	3.7×10 <sup>-3</sup> – 1.0		neg.	3.6×	10 <sup>-3</sup>	4.8×10 <sup>-5</sup> – 6.3×10 <sup>-3</sup>	2.4×10 <sup>-4</sup> – 2.9×10 <sup>-3</sup>				2.4×10 <sup>-4</sup> – 2.9×10 <sup>-3</sup>	1.6×10 <sup>-5</sup>			
esyl pł	Soil (mg/kg wet weight)	neg.		neg.	0.0	)3	4.6×10 <sup>-4</sup> – 0.05	1.9×10 <sup>-3</sup> – 0.02				1.9×10 <sup>-3</sup> – 0.02	2.14×10 <sup>-4</sup>			2.4×10 <sup>-5</sup>
Tricresyl phosphate	Secondary poisoning – fish (mg/kg)	0.01 – 0.04		neg.	0.1	2	4.7×10 <sup>-3</sup> – 0.21	5.0×10 <sup>-3</sup> – 9.3×10 <sup>-3</sup>				0.01 – 0.1	4.93×10 <sup>-3</sup>			3.8×10 <sup>-4</sup>
	Secondary poisoning – earthworm (mg/kg)	neg.		neg.	0.0	08	2.0×10 <sup>-3</sup> – 0.13	6.0×10 <sup>-3</sup> – 0.06				6.1×10 <sup>-3</sup> – 0.06	1.3×10 <sup>-3</sup>			

Table 3.4 continued.

-	Media									PEC							
Product		Production	Textile coating	Adhesives	Paints	Pigment dispersions	Printed circuit boards	PVC	Polyurethane	Thermoset resins	Thermoplastic/ stryrenic resins	Rubber	Photographic film	Lubricant additive	Hydraulic fluid	Power generation fluid	Regional sources
-	Water (µg/l)	1.06											<del>_</del>			0.09	0.02
	Sediment (mg/kg wet weight)	0.20														0.02	6.9×10 <sup>-3</sup>
Tri	WWTP (mg/l)	0.04														0.70	
kyleny	Soil (mg/kg wet weight)	9.0×10 <sup>-6</sup>														0.02	2.2x10 <sup>-6</sup>
Trixylenyl phosphate	Secondary poisoning – fish (mg/kg)	0.85														0.09	5.5×10 <sup>-4</sup>
W	Secondary poisoning – earthworm (mg/kg)	8.6×10 <sup>-3</sup>														0.29	

Table 3.4 continued.

	Media								PEC								
Product		Production	Textile coating	Adhesives	Paints	Pigment dispersions	Printed circuit boards	PVC	Polyurethane	Thermoset resins	Thermoplastic/ stryrenic resins	Rubber	Photographic film	Lubricant additive	Hydraulic fluid	Power generation fluid	Regional sources
	Water (µg/l)	0.08	0.25 - 0.84					0.46 – 1.19	0.31 – 1.19					0.03	0.03	0.04	0.02
Tertb	Sediment (mg/kg wet weight)	7.9×10 <sup>-3</sup>	0.03 – 0.09					0.05 – 0.13	0.03 – 0.13					2.9×10 <sup>-3</sup>	3.0×10 <sup>-3</sup>	4.5×10 <sup>-3</sup>	2.1×10 <sup>-3</sup>
utyl pł	WWTP (mg/l)	2.3×10 <sup>-3</sup>	2.4×10 <sup>-3</sup> – 8.3×10 <sup>-3</sup>					4.4×10 <sup>-3</sup> – 0.01	3.0×10 <sup>-3</sup> – 0.01					7.9×10 <sup>-5</sup>	9.0×10 <sup>-5</sup>	2.3×10 <sup>-4</sup>	
ıenyl di	Soil (mg/kg wet weight)	neg.	0.01 – 0.04					0.02 – 0.05	0.01 – 0.05					3.5×10 <sup>-4</sup>	4.1×10 <sup>-4</sup>	1.1×10 <sup>-3</sup>	2.6×10 <sup>-6</sup> - 1.8×10 <sup>-3</sup>
Tertbutyl phenyl diphenyl phosphate	Secondary poisoning – fish (mg/kg)	0.04	0.02 – 0.28					0.08 - 0.39	0.11 – 0.39					0.02	0.02	0.02	1.0^10
າosphate	Secondary poisoning – earthworm (mg/kg)	neg.	0.05 – 0.19					0.10 – 0.27	0.07 – 0.27					1.9×10 <sup>-3</sup>	2.1×10 <sup>-3</sup>	5.6×10 <sup>-3</sup>	

Table 3.4 continued.

	Media								PEC								
Product		Production	Textile coating	Adhesives	Paints	Pigment dispersions	Printed circuit boards	PVC	Polyurethane	Thermoset resins	Thermoplastic/ stryrenic resins	Rubber	Photographic film	Lubricant additive	Hydraulic fluid	Power generation fluid	Regional sources
	Water (µg/l)	3.39	0.67 – 1.34	neg.	0.53 – 19.8	0.58		0.37 – 2.68	0.5 – 2.32		0.35 – 0.47			0.35	0.34		0.34
Isoprop	Sediment (mg/kg wet weight)	0.43	0.09 – 0.17	neg.	0.07 – 2.53	0.07		0.05 – 0.34	0.06 – 0.30		0.04 – 0.06			0.04	0.04		0.06
ylpher	WWTP (mg/l)	0.12	3.4×10 <sup>-3</sup> – 0.01	neg.	2.0×10 <sup>-3</sup> - 0.20	2.5×10 <sup>-3</sup>		1.0×10 <sup>-3</sup> – 0.02	1.7×10 <sup>-3</sup> – 0.02		1.1×10 <sup>-4</sup> – 1.4×10 <sup>-3</sup>			8.9×10 <sup>-5</sup>	4.9×10 <sup>-5</sup>		
ıyl dip	Soil (mg/kg wet weight)	neg.	0.07 – 0.21	neg.	0.04 – 4.11	0.05		6.1×10 <sup>-3</sup> – 0.50	0.04- 0.42		2.6×10 <sup>-3</sup> – 0.03			2.0×10 <sup>-3</sup>	1.2×10 <sup>-3</sup>		1.6×10 <sup>-4</sup> – 0.13
lsopropylphenyl diphenyl phosphate	Secondary poisoning – fish (mg/kg)	1.02	0.27 – 0.42	neg.	0.24 – 4.69	0.20		0.19 – 0.73	0.23 – 0.65		0.19 – 0.22			0.19	0.19		
osphate	Secondary poisoning – earthworm (mg/kg)	0.03	0.73 – 2.12	neg.	0.44 – 40.6	0.54		0.08 – 4.93	0.38 – 4.17		0.05 – 0.3			0.04	0.03		

Table 3.4 continued.

	Media								PEC								
Product		Production	Textile coating	Adhesives	Paints	Pigment dispersions	Printed circuit boards	PVC	Polyurethane	Thermoset resins	Thermoplastic/ stryrenic resins	Rubber	Photographic film	Lubricant additive	Hydraulic fluid	Power generation fluid	Regional sources
	Water (µg/I)	1.33	0.40 – 1.08	neg.	0.27 – 0.61	0.81		0.10 – 1.21	0.13 – 0.88					0.07	0.10	0.07	0.07
Tris(is	Sediment (mg/kg wet weight)	0.42	0.13 – 0.34	neg.	0.08 – 0.19	0.25		0.03 – 0.38	0.04 – 0.28					0.02	0.03	0.02	0.04
oprop	WWTP (mg/l)	0.05	3.4×10 <sup>-3</sup> – 0.01	neg.	2.1×10 <sup>-3</sup> – 5.5×10 <sup>-3</sup>	7.6×10 <sup>-3</sup>		6.9×10 <sup>-4</sup> − 0.01	6.9×10 <sup>-4</sup> – 8.3×10 <sup>-3</sup>					5.3×10 <sup>-5</sup>	3.2×10 <sup>-4</sup>	5.6×10 <sup>-5</sup>	
ylpheı	Soil (mg/kg wet weight)	neg.	0.18 – 0.55	neg.	0.11 – 0.29	0.40		0.02 - 0.62	0.04 - 0.44					2.9×10 <sup>-3</sup>	0.02	4.1×10 <sup>-3</sup>	6.3×10 <sup>-5</sup> – 0.08
Tris(isopropylphenyl) phosphate	Secondary poisoning – fish (mg/kg)	1.34	0.18 – 0.27	neg.	0.16 – 0.57	0.74		0.16 – 1.07	0.14 -0.28					0.14	0.13	0.14	
sphate	Secondary poisoning – earthworm (mg/kg)	0.01	4.79 – 14.3	neg.	2.87 – 7.66	10.5		0.49 – 16.2	1.0 – 11.5					0.09	0.46	0.12	

Table 3.4 continued.

	Media								PEC								
Product	_	Production	Textile coating	Adhesives	Paints	Pigment dispersions	Printed circuit boards	PVC	Polyurethane	Thermoset resins	Thermoplastic/ stryrenic resins	Rubber	Photographic film	Lubricant additive	Hydraulic fluid	Power generation fluid	Regional sources
	Water (µg/l)	0.19	0.64 – 6.49	neg.	0.25-15.1	1.81		0.76 – 21.2	1.34 – 2.98			1.34 – 2.98	1.34 – 2.98				0.17
2-Ethylhexyl	Sediment (mg/kg wet weight)	0.04	0.13 – 1.35	neg.	0.05-3.14	0.38		0.16 – 4.4	0.28 - 0.62			0.28 - 0.62	0.28 – 0.62				0.04
/lhexy	WWTP (mg/l)	1	4.8×10 <sup>-3</sup> – 0.06	neg.	7.6×10 <sup>-4</sup> – 0.15	0.02		5.9×10 <sup>-3</sup> – 0.21	0.01 – 0.03			0.01 – 0.03	0.01 – 0.03				
l diphenyl	Soil (mg/kg wet weight)	neg.	0.07 – 0.92	neg.	0.01 – 2.17	0.24		0.09 - 3.06	0.17 – 0.41			0.17 – 0.41	0.17 – 0.41				2.9×10 <sup>-4</sup> – 0.02
enyl pho	Secondary poisoning – fish (mg/kg)	0.17	0.16 – 2.59	neg.	0.16 – 5.91	0.79		0.16 – 8.24	0.16 – 1.24			0.61 – 1.24	0.71 – 1.24				
phosphate	Secondary poisoning – earthworm (mg/kg)	0.01	1.0 – 13.4	neg.	0.17 – 31.8	3.49		1.25 – 44.7	2.5 – 5.97			2.5 – 5.97	2.5 – 5.97				

Table 3.4 continued.

	Media								PEC								
Product		Production	Textile coating	Adhesives	Paints	Pigment dispersions	Printed circuit boards	PVC	Polyurethane	Thermoset resins	Thermoplastic/ stryrenic resins	Rubber	Photographic film	Lubricant additive	Hydraulic fluid	Power generation fluid	Regional sources
	Water (µg/l)	n/aª	0.52 – 1.4		0.70 – 7.22	1.49		0.39 – 10.6	0.61 – 1.93			0.61 – 1.93					0.17
Isod	Sediment (mg/kg wet weight)	n/a <sup>a</sup>	0.08 – 0.21		0.10 – 1.08	0.22		0.06 – 1.58	0.09 – 0.29			0.09 – 0.29					0.04
ecyl c	WWTP (mg/l)	n/aª	3.6×10 <sup>-3</sup> – 0.01		5.4×10 <sup>-3</sup> – 0.07	0.01		2.2×10 <sup>-3</sup> – 0.11	4.5×10 <sup>-3</sup> – 0.02			4.5×10 <sup>-3</sup> – 0.02					
liphen	Soil (mg/kg wet weight)	1.4×10 <sup>-3</sup>	0.10 – 0.36		0.15 – 2.04	0.38		0.07 – 3.02	0.13 – 0.51			0.13 – 0.51					9.7×10 <sup>-4</sup> – 0.08
lsodecyl diphenyl phosphate	Secondary poisoning – fish (mg/kg)	n/aª	0.06 – 0.23		0.06 – 1.03	0.24		0.06 – 1.49	0.06 – 0.3			0.06 – 0.3					
hate	Secondary poisoning – earthworm (mg/kg)	0.03	1.26 – 4.36		1.87 – 24.7	4.65		0.80 – 36.5	1.58 – 6.2			1.58 – 6.2					

Notes: a) Production not included since the production sites only discharge to a marine environment.

Table 3.4 continued.

	Media							F	PEC								
Product		Production	Textile coating	Adhesives	Paints	Pigment dispersions	Printed circuit boards	PVC	Polyurethane	Thermoset resins	Thermoplastic/ stryrenic resins	Rubber	Photographic film	Lubricant additive	Hydraulic fluid	Power generation fluid	Regional sources
	Water (µg/l)	0.07 - 3.55			0.32 -0.45	1.52		0.08 - 0.37	0.19 - 1.66		1.58 - 18.2						0.05
Tetrap	Sediment (mg/kg wet weight)	0.01 - 0.57			0.05 – 0.07	0.24		0.01 – 0.06	0.03 – 0.27		0.25 – 2.91						0.02
henyl	WWTP (mg/l)	1.2×10 <sup>-3</sup> – 0.14			2.7×10 <sup>-3</sup> – 4.1×10 <sup>-3</sup>	0.01		2.7×10 <sup>-4</sup> – 3.2×10 <sup>-3</sup>	1.4×10 <sup>-3</sup> – 0.02		0.02 – 0.18						
resorc	Soil (mg/kg wet weight)	1.5×10 <sup>-4</sup> – 2.1×10 <sup>-4</sup>			0.06 - 0.09	0.33		6.1×10 <sup>-3</sup> – 0.07	0.03 - 0.36		0.34 – 4.03						1.5×10 <sup>-4</sup> – 0.14
Tetraphenylresorcinol diphosphate	Secondary poisoning – fish (mg/kg)	0.06 – 1.68			0.05 – 0.16	0.64		0.05 – 0.18	0.05 – 0.69		0.66 – 7.28						
าosphate	Secondary poisoning – earthworm (mg/kg)	4.0×10 <sup>-3</sup> – 4.9×10 <sup>-3</sup>			0.77 – 1.16	4.23		0.08 - 0.93	0.39 – 4.62		4.42 - 52.3						

# 3.2 Environmental effects

# 3.2.1 Aquatic compartment (including sediment and waste water treatment plant)

The amount of aquatic toxicity data available for the aryl phosphate esters is variable and so a read-across approach was used to fill in gaps in the database (this is discussed in Annex B). This ignores the possible influence of isomerism on toxic potency, which has been observed in the mammalian toxicity datasets of some substances for a few end points. Whilst this is also a possible issue for aquatic effects, the limited data do not allow any inferences to be made about its significance.

Table 3.5 Summary of predicted no effect concentrations (PNECs)

Substance		Predicted no	effect concent	ration (PNE	C)
-	Surface water (µg/I)ª	Sediment (mg/kg wet wt.)	Microorgan isms (mg/l)	Soil (mg/kg wet wt.)	Secondary poisoning (mg/kg food)
Triphenyl phosphate	0.74	0.16	0.51	0.13	3.33
Cresyl diphenyl phosphate	1.4	0.074	>100	0.059	0.8
Tricresyl phosphate	0.032	0.0033 <sup>b</sup>	>100	0.0027 <sup>b</sup>	1.7
Trixylenyl phosphate	0.7	0.13 <sup>b</sup>	160	0.105	Insufficient data
Tertbutylphenyl diphenyl phosphate	1	0.104 <sup>b</sup>	Insufficient data	0.084 <sup>b</sup>	4.4
Isopropylphenyl diphenyl phosphate	0.6	0.077 <sup>b</sup>	>1	0.062 <sup>b</sup>	1.8
Tris(isopropyl- phenyl) phosphate	0.6	0.188 <sup>b</sup>	>1	0.153 <sup>b</sup>	Insufficient data
2-Ethylhexyl diphenyl phosphate	1.8	0.373 <sup>b</sup>	>100	0.302 <sup>b</sup>	1.1
Isodecyl diphenyl phosphate	0.4	0.059 <sup>b</sup>	3	0.048 <sup>b</sup>	0.52
Tetraphenyl resorcinol diphosphate	2.1	0.336 <sup>b</sup>	122	0.272 <sup>b</sup>	220

Notes:

- a) PNECs based on measured toxicity data are shown in bold; those based on predicted data are shown in normal font.
- b) These substances have log K<sub>ow</sub> values above five and so the resulting PEC/PNEC ratios have been increased by a factor of 10 to take into account the possibility of ingestion of sediment-bound substance.

The predicted no effect concentrations (PNECs) for surface water given in Table 3.5 were derived from either the lowest experimental no observed effect concentration

(NOEC) (marked in Table 3.5 in bold) or, for substances where long-term data were not available for fish, invertebrates and/or algae, the read-across predicted lowest NOEC (normal text in Table 3.5). In most cases an assessment factor of 10 was used on the lowest NOEC to derive the PNEC; the exception is triphenyl phosphate, where an assessment factor of 50 was used on the lower of two experimental NOEC values.

All of the PNECs are derived from data (measured or predicted) for fish or Daphnia. The measured (Table 3.2) and predicted toxicity data for algae suggest that they are less sensitive than fish or Daphnia. In general, Daphnia tend to be more sensitive than fish, but there is at least one exception to this. The analysis in Annex B suggests that fish have a similar sensitivity to most of the substances in these assessments (when expressed on a molar basis).

No toxicity data are available for sediment-dwelling organisms and so a provisional PNEC was calculated using the equilibrium partitioning method outlined in the TGD (see Table 3.5).

The aryl phosphates generally show low toxicity to microorganisms. The PNECs derived for microorganisms are also summarised in Table 3.5.

# 3.2.2 Terrestrial compartment

Few toxicity studies are available on soil-dwelling organisms. In the absence of sufficient information, PNECs for soil were estimated using the equilibrium partitioning method and these are summarised in Table 3.5. Again, as for sediment, PEC/PNEC ratios were increased by a factor of 10 to take account of possible direct ingestion of soil-bound residues.

# 3.2.3 Atmosphere

No toxicity data are available for air exposure of relevant organisms. The low vapour pressure of the substances means that their potential contribution to atmospheric effects such as global warming and acid rain is likely to be small. In addition, as they do not contain halogen atoms they will not contribute to ozone depletion.

# 3.2.4 Non-compartment specific effects relevant to the food chain (secondary poisoning)

PNEC<sub>oral</sub> values for secondary poisoning are summarised in Table 3.5. They reflect not only the differences in toxicity of the various substances but also the different amounts and types of information available (which affects the assessment factor used). The underlying mammalian and avian toxicology data behind these PNECs were reviewed as part of this project, although there are significant gaps for some substances, and a number of questions remain to be answered for others.

# 3.2.5 Hazard classification

# Health

None of the substances in this series is currently included in Annex I of Directive 67/548/EEC. Proposals for classification were developed based on the assessment of

available data. Table 3.6 summarises these proposals, and also indicates those endpoints for which classification is not required, and those where there are insufficient data to make a decision.

# Environment

Triphenyl phosphate is the only substance currently included on Annex I, with a classification of R50/53. Based on the current assessments, the same classification is proposed for the other substances, with the exception of tris(isopropylphenyl) phosphate, for which R53 is proposed, and trixylenyl phosphate, for which R51/53 is proposed.

Table 3.6 Summary of human health classification conclusions

Endpoint	2EHDPP	CDPP	IDDPP	IPTPP	TBPDPP	TCP	TPP	TPRDP	TXP
Acute toxicity	R20: harmful by inhalation <sup>a</sup>	-	-	-	-	Toxic – oral Harmful – dermal, inhalation	-	-	-
Skin/eye irritation	-	-	ID	ID (eye)	-	-	-	-	-
Corrosivity	-	-	-	-	-	-	-	-	-
Sensitisation	-	ID	-	-	ID	Yes	-	ID	ID
Repeat dose	-	Xn R48 <sup>a</sup>	ID	Xn R48	-	Xn R48	-	-	ID
Reproductive toxicity	-	Cat 2 R60	ID	ID	-	Cat 2	-	-	ID
Developmental toxicity	-	-	-	ID	-	-	-	-	ID
Mutagenicity	-	-	ID	-	-	-	ID	-	ID
Carcinogenicity	-	ID	ID	ID	ID	-	ID	ID	ID

a – dependent on further clarification of test results

2EHDPP – 2-ethylhexyl diphenyl phosphate; CDPP – cresyl diphenyl phosphate; IDDPP – isodecyl diphenyl phosphate; IPTPP – isopropylated triphenyl phosphate; TBPDPP – tertbutylphenyl diphenyl phosphate; TCP – tricresyl phosphate; TPP – triphenyl phosphate; TPP – tetraphenyl resorcinol diphosphate; TXP – trixylenyl phosphate.

ID – insufficient data at present

# 3.3 Environmental risk characterisation

The realistic worst case PEC/PNEC ratios are summarised in Figures 3.2 to 3.11. In order to display all of the PEC/PNEC ratios for each substance, the figures use a logarithmic scale. On this scale, a PEC/PNEC ratio of one acts as the origin; a bar extending above this line indicates a worst case PEC/PNEC ratio of above one, that is a risk, and a bar extending below this line indicates a PEC/PNEC ratio of below one (low concern). All PEC/PNEC ratios below 0.01 have been set to 0.01 to make the data presented in Figures 3.2 to 3.11 clearer and easier to interpret. Figure 3.1 presents the key to the protection goals in the charts.

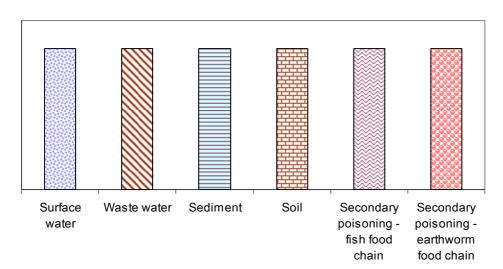


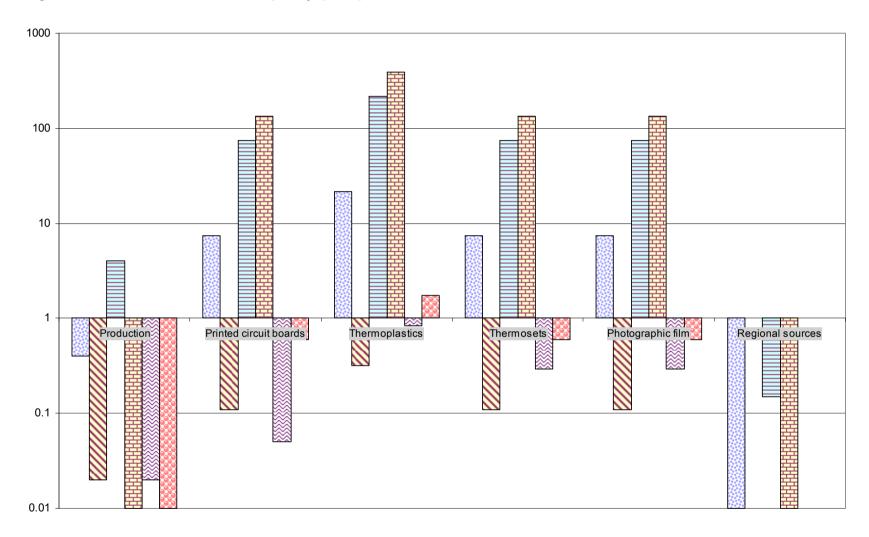
Figure 3.1 Key to risk characterisation charts

The ratios shown are the highest value for each use; in some cases, there are a number of steps involved in a use and there may not be a risk for all of the steps. In the case of PVC, some substances are used in a range of product types. These were assessed individually in the individual assessment reports, but were combined under one heading here for simplicity.

The approach taken to estimate releases to the environment underlying the PECs is based on the best available information. The estimates take account of information supplied by companies on amounts used by customers. The emission estimates are largely based on information for the particular industry areas, as included in emission scenario documents, but not on information on the aryl phosphates themselves. It is therefore possible that the exposure estimation could be improved.

All substances show some PEC/PNEC ratios above one and suggestions for further work to refine these assessments are given in Section 4.







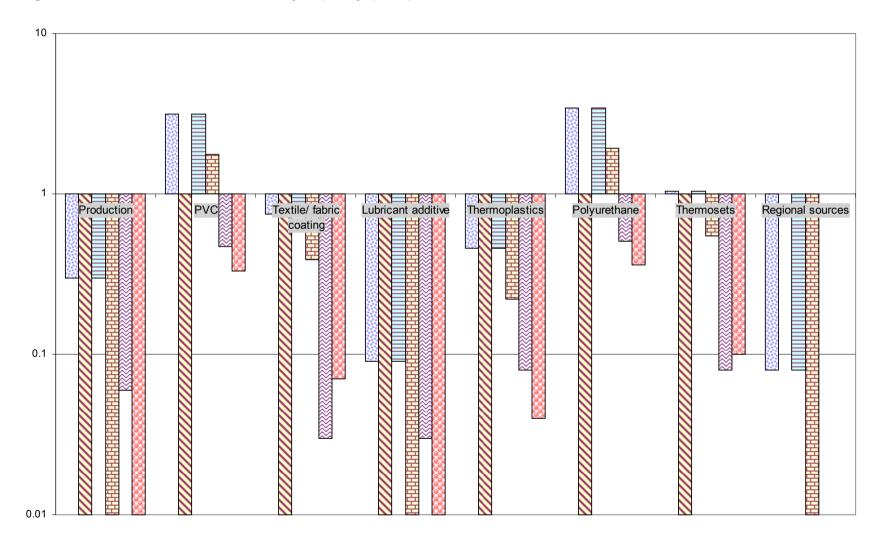


Figure 3.4 PEC/PNEC ratios for tricresyl phosphate

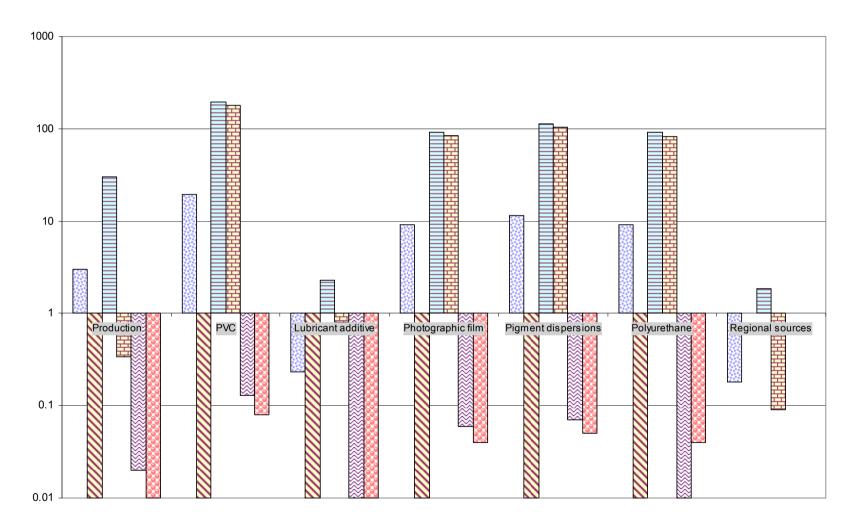
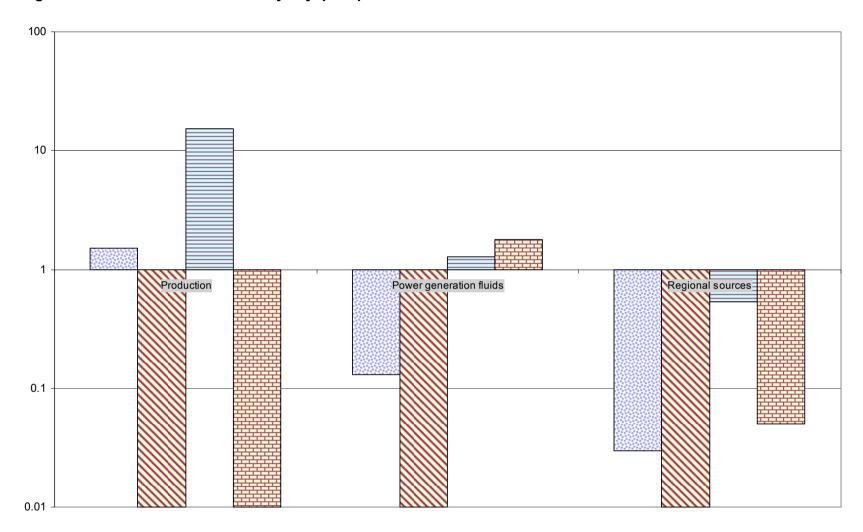


Figure 3.5 PEC/PNEC ratios for trixylenyl phosphate



Note: There are insufficient data to derive a PNEC for secondary poisoning. A risk characterisation for secondary poisoning has not been carried out.

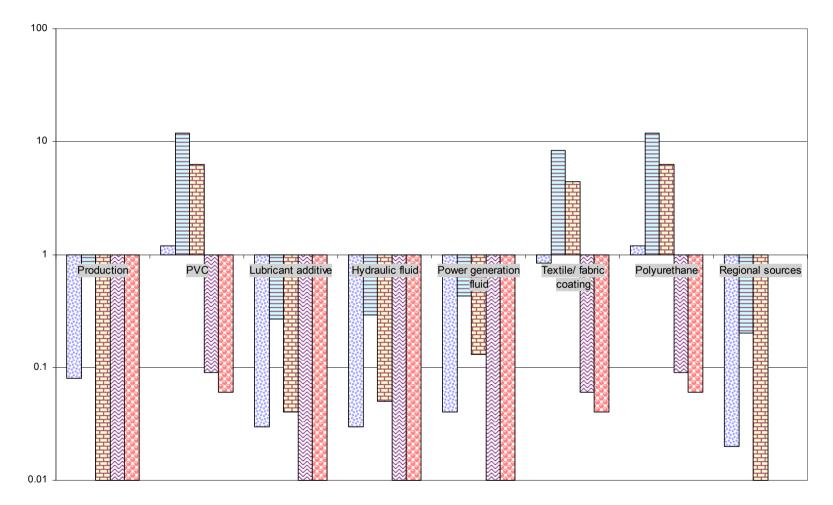


Figure 3.6 PEC/PNEC ratios for tertbutylphenyl diphenyl phosphate

Note: There are insufficient data to derive a PNEC microorganism for sewage treatment processes. A risk characterisation for waste water has not been carried out.

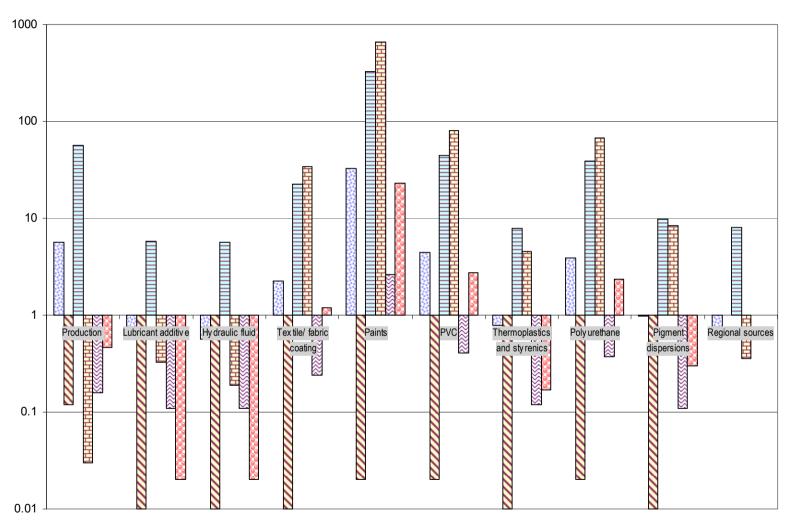
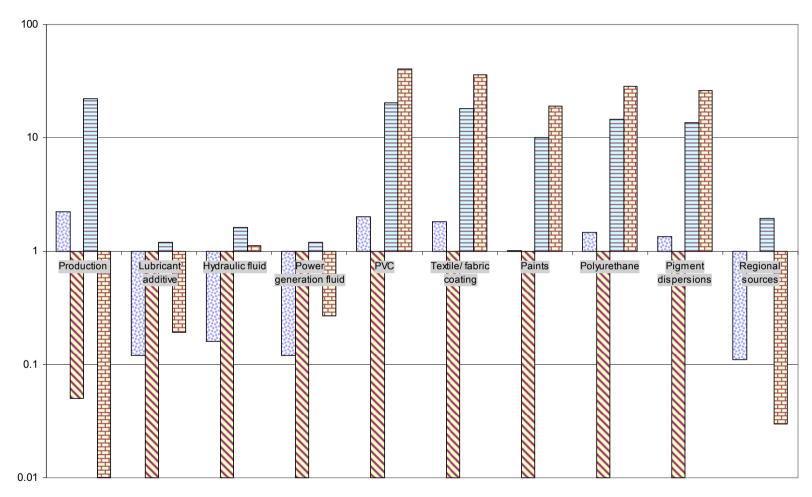


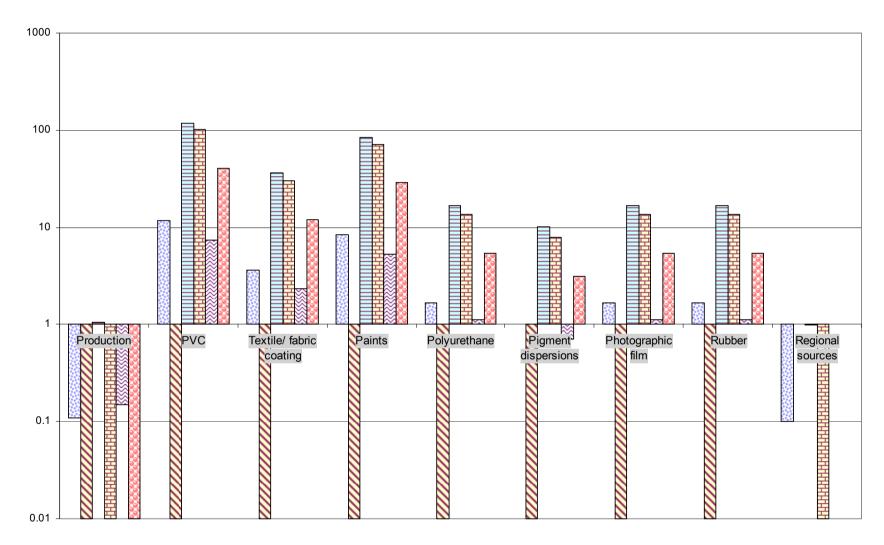
Figure 3.7 PEC/PNEC ratios for isopropylphenyl diphenyl phosphate

Figure 3.8 PEC/PNEC ratios for tris(isopropylphenyl) phosphate



Note: There are insufficient data to derive a PNEC for secondary poisoning. A risk characterisation for secondary poisoning has not been carried out.







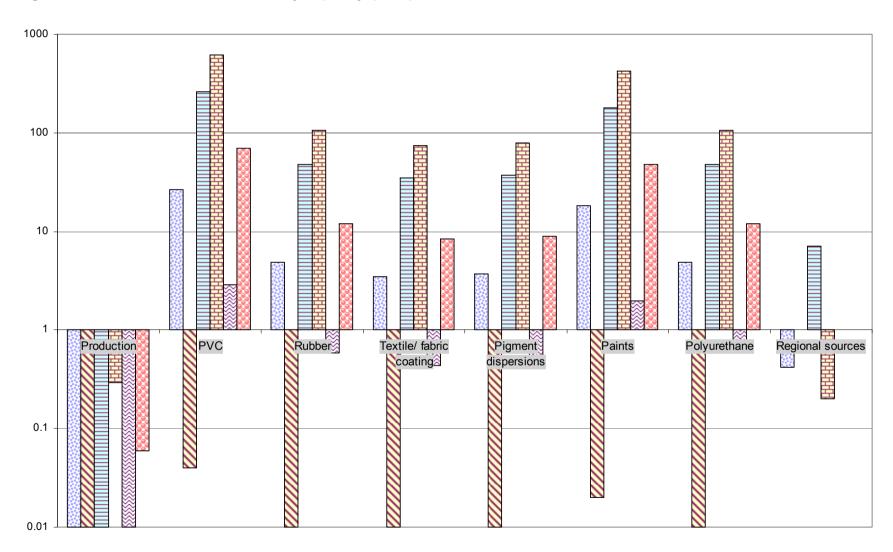
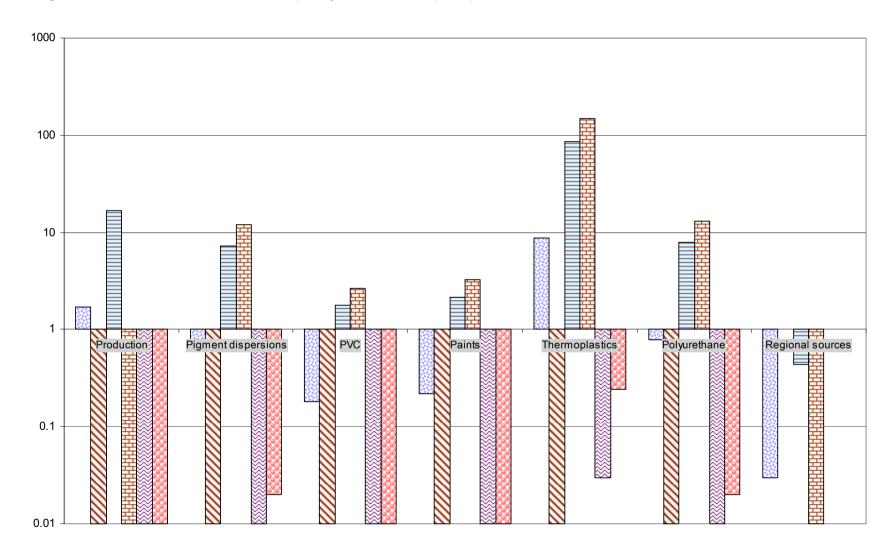


Figure 3.11 PEC/PNEC ratios for tetraphenyl resorcinol diphosphate



#### 3.3.1 Considerations for marine risk assessment<sup>2</sup>

This section considers the properties of the aryl phosphates against the persistence, bioaccumulation and toxicity (PBT) criteria in the TGD. These are summarised below:

P vP	Half-life in fresh water over 40 days Half-life in marine water over 60 days Half-life in freshwater sediment over 120 days Half-life in marine sediment over 180 days Half-life in fresh water or marine water over 60 days
	Half-life in freshwater or marine sediment over 180 days
B vB	BCF over 2,000 l/kg BCF over 5,000 l/kg
Т	Chronic aquatic NOEC under 0.01 mg/l, or chronic mammalian toxicity

The relevant properties for the individual substances and the results of the PBT assessment are shown in

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<sup>&</sup>lt;sup>2</sup> Marine risk assessment results are included in the individual risk assessment reports. In general the risk characterisation ratios for marine waters and sediments are higher than those calculated for freshwater, as the PNECs are 10 times lower while the PEC values are not reduced to the same degree due to the assumption of no waste water treatment plant for marine discharges. The concentrations in predators tend to be lower, so the conclusions for the marine food chain do not show as many risks as for the freshwater food chain.

#### Table 3.7.

With regard to the P and vP criteria, it is clear that all of the aryl phosphates considered in this assessment have the potential to be degraded (by biotic and abiotic processes) in the environment. However, for most substances there is a lack of simulation studies from which to estimate a reliable degradation half-life for freshwater, marine water, freshwater sediment or marine water sediment, and so the assessment of whether the substance may or may not meet the P or vP criteria is based on screening data from standard ready and inherent biodegradation tests. The TGD indicates that such data can be used in a screening assessment to decide if the substance is not P (if the substance is readily biodegradable or inherently biodegradable meeting specific criteria) or whether further testing may be needed to determine if the substance is actually P or vP (if the substance is inherently biodegradable not meeting specific criteria or not readily or inherently biodegradable).

The decision is straightforward for those substances that are readily biodegradable. The situation for the other substances is not so clear. There may be indications that acclimated organisms are able to degrade them, or that relatively rapid primary degradation takes place in river die-away tests. For the estimation of exposure in the risk assessment, the choice was made to interpret these results as being equivalent to inherently degradable meeting the specific criteria (so that the biodegradation rates in the environment are not zero). If a lack of degradability were assumed, then there would be no biodegradation in the environment which clearly does not fit with the observed results. This approach was chosen because the available data do not allow degradation rates to be estimated for each substance in each compartment, so default rates are used instead.

Table 3.7 Screening PBT assessment

Substance	Biodegradation classification <sup>a</sup>	BCF for fish (I/kg)	Chronic NOEC (mg/l)	Initial PBT evaluation
Triphenyl	Readily	420	0.037	Not P
phosphate	biodegradable		(0.032	Not B
			estimated)	Not T
Tricresyl	Readily	800	0.00032	Not P
phosphate	biodegradable			Not B
				T
Cresyl diphenyl	Ready	200	0.014	Not P
phosphate	biodegradable		(estimated)	Not B
				T (see text)
Trixylenyl phosphate	Inherently biodegradable (not possible to determine if specific criteria are met)	~1,900	0.007 (estimated)	Meets the first stage screening criteria for P/vP <sup>b</sup> Meets the first stage screening criteria for B (borderline)
	•			Possibly T
Isopropyl	Readily	564	0.006	Not P
phenyl diphenyl phosphate	biodegradable			Not B
				Т
Tris(isopropyl- phenyl)	Inherently biodegradable	1,986 (est.d)	0.006 (estimated)	Meets the first stage screening criteria for P/vP <sup>t</sup>
phosphate	(not possible to determine if specific criteria are met)			Meets the first stage screening criteria for B (borderline)
	•			Possibly T (see text)
Tertbutylphenyl	Readily	778	0.010	Not P
diphenyl phosphate	biodegradable			Not B
•				Borderline T
Tetraphenyl resorcinol diphosphate	Inherently biodegradable (not possible to	969 (est.d)	0.014	Meets the first stage screening criteria for P/vP <sup>t</sup>
шрпоэрнасе	determine if specific criteria are met)			Not B Not T
2-Ethylhexyl-	Readily	934	0.018	Not P
diphenyl	biodegradable			Not B
phosphate				Not T
lsodecyl- diphenyl	Inherently biodegradable	335	0.004	Meets the first stage screening criteria for P or vF
phosphate	(not possible to determine if specific criteria are met)			Not B T

Notes:

- a) Abiotic hydrolysis may also be important for the marine environment under the timescales being considered (the pH of seawater is typically around 8).
- b) The assessment is based on the behaviour in standard ready and inherent biodegradation tests. Further testing would be needed to determine an actual mineralization half-life in surface water or sediment to provide a definitive assignment.

The situation with regard to the PBT assessment is different. There are no inherent tests carried out to specified guidelines with sufficient information to decide whether they meet the specific criteria for those guidelines. Hence on the basis of the available data it is not possible to conclude that these substances do not meet the P criteria (although the evidence suggests they do not). This applies to five substances in the group, and the conclusion is of meeting the first stage screening criteria for P. This analysis does not take possible hydrolysis half-lives into account.

BCF values for fish derived for all substances in this series are below 2,000 l/kg (see

Table 3.7 for details). On this basis, none of the aryl phosphates assessed meet the B or vB criteria. However, trixylenyl phosphate and tris(isopropylphenyl) phosphate have BCF values of 1,900 and 1,986 kg/l, respectively, which are close to the B threshold of 2,000 kg/l. For tris(isopropylphenyl) phosphate, the BCF was estimated by looking at available data for all of the substances and was considered to be subject to some uncertainty. Some measured values for this substance are also above the threshold value. The value for trixylenyl phosphate is an experimental value, but the study noted that steady state had not been fully reached. As the value is close to the threshold, there is some uncertainty in relation to the criterion. Therefore, for these two substances the preliminary conclusion is that they meet the screening criterion for B.

Chronic NOEC values were estimated for tetraphenyl resorcinol diphosphate and cresyl diphenyl phosphate. Neither substance meets the T criterion. The lowest measured chronic NOEC of 0.037 mg/l for triphenyl phosphate compares well with the estimated value of 0.032 mg/l; the T criterion is not met. Estimated NOECs for trixylenyl phosphate and tris(isopropylphenyl) phosphate indicate that these substances are possibly toxic. The lowest measured chronic NOEC values for tricresyl phosphate, isopropyl phenyl diphenyl phosphate and isodecyl diphenyl phosphate are all under 0.01 mg/l, and so the T criterion is met for these. 2-Ethylhexyldiphenyl phosphate is not considered to meet the T criterion (measured NOEC over 0.01 mg/l). The lowest measured chronic NOEC for tertbutylphenyl diphenyl phosphate is 0.01 mg/l, so this substance is considered borderline for toxicity.

Regarding mammalian toxicity, Table 3.6 suggests that tricresyl phosphate and cresyl diphenyl phosphate should be classified as Category 2 reprotoxins, and isopropylated triphenyl phosphate should be classified with the risk phrase R48. These indications of chronic effects trigger the T criterion. In addition, a lack of relevant toxicological information for several of the substances means that this could be kept under review.

The overall conclusions of the PBT assessment are that two of the substances cannot currently be excluded as meeting the PBT criteria. These are trixylenyl phosphate and tris(isopropylphenyl) phosphate.

#### 3.3.2 Human exposure through the environment

An assessment of the potential risks to humans exposed to aryl phosphates through the environment was carried out. The results are summarised in Table 3.8.

Table 3.8 Summary of potential risks for humans exposed through the environment

Life cycle step	2EHDPP	CDPP	IDDPP	TCP	TPP	TPRDP
Production	-	-	-	-	-	-
Adhesives	-	-	na	-	na	na
Lubricants	na	-	na	na	na	na
Paints	*	na	*	na	na	-
Photographic film	*	na	na	-	-	na
Pigment dispersions	-	na	*	-	na	-
Polyurethane	*	-	*	-	na	-
Printed circuit boards	na	na	na	na	-	na
PVC	*	-	*	-	na	-
Rubber	*	na	*	na	na	na
Textiles/fabric coating	*	-	*	na	na	na
Thermoplastics/styrenics	na	-	na	na	-	-
Thermosets and epoxy resins	na	-	na	na	-	na

Notes:

\* - potential risk identified

na – not a use for this substance

2EHDPP – 2-ethylhexyl diphenyl phosphate; CDPP – cresyl diphenyl phosphate; IDDPP – isodecyl diphenyl phosphate; TCP – tricresyl phosphate; TPP – triphenyl phosphate; TPRDP – tetraphenyl resorcinol diphosphate.

No assessment is currently possible for isopropylated triphenyl phosphate, tertbutylphenyl diphenyl phosphate and trixylenyl phosphate due to inadequate toxicological data.

### 4 Conclusions and further information needs

The risk evaluation reports have identified a number of areas where further information would be useful to determine more reliably whether a risk to the environment exists.

The information needs can be broadly divided into six main areas as follows.

- Further information on exposure.
- Further information on toxicity to aquatic organisms.
- Further information on toxicity to sediment organisms.
- Further information on toxicity to soil organisms.
- Further information on degradation in the environment.
- Further evaluation of the available avian and mammalian toxicity data.

#### 4.1 Further information on exposure

Further information on exposure is needed for most of the aryl phosphate esters considered. In terms of the original aims of the project (to investigate risks from the use of aryl phosphates in applications where they may be used as possible replacements for other flame retardants), the exposure information that would be most useful would include the following applications:

- use in PVC:
- use in thermoplastics/styrenics;
- use in printed circuit boards;
- use in epoxy resins;
- use in polyurethane;
- use in rubber:
- use in paints;
- use in textile coatings.

In particular, more specific data could be provided on emissions from sites using the substances in the production of these materials (or making products from them). It would be useful if this were accompanied by information on emission control measures and cleaning procedures, and on the amounts used at representative sites<sup>3</sup> (on a realistic worst case basis).

As well as information on local emissions from processing sites, information on the emissions of aryl phosphates from treated articles during their service life and disposal would be useful, because these make a significant contribution to the regional emissions. The calculated  $PEC_{regional}$  is crucial in some assessments, particularly for the isopropylated phenyl phosphates.

The current assessments make use of information from a number of sources in estimating emissions to the environment. Most of the uses relate to different types of plastics. For these, an ESD on plastics additives has been used. This covers raw materials handling, compounding and conversion, as well as the service life of articles.

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<sup>&</sup>lt;sup>3</sup> Information on this aspect was provided by the manufacturers for these assessments, and so refining this part of the exposure assessment may not lead to major changes.

Most of the emission factors used in the ESD are derived from information on phthalate esters (mainly di-ethylhexyl phthalate). Hence the estimates are not based on data for the actual aryl phosphate substances, and so specific information on releases of the substances could refine the assessments. However, the methods in the ESD have been used for a number of other risk assessments, and so a significant amount of information (such as measured emissions from a representative sample of plants using the substance) would be needed to replace the ESD values completely. Additional information on waste treatment and cleaning at a small number of user sites was provided and this information did not contradict the assumptions made on the basis of the ESD.

It would not be necessary to obtain information on every plastics application. Where there are common steps, for example in raw material handling, information from a subset of the applications could be read-across to the others.

Some areas such as textiles make use of information from assessments on other substances under the Existing Substances Regulation. Again, the estimates are not based on information on specific substances, but do make use of actual data from the industry or use area.

The assessment of lubricants and hydraulic fluid applications makes use of another ESD, on lubricants and additives. The methods are a mixture of theoretical calculations and collected data on losses. Similar comments to those on plastics apply here. These uses do not generally show risks to the same extent as for plastics.

## 4.2 Further information on toxicity to aquatic organisms

Risks are shown for the aquatic compartment in a large number of cases, and so consideration should be given to refining the PNEC where possible. In addition, the PNEC for surface water is currently important for the sediment and soil assessments as the PNECs for these compartments are estimated by equilibrium partitioning.

In terms of refining the aquatic PNECs, there is limited scope for changes for most of the substances. This is because the approach in the risk assessments does not follow the TGD exactly, but applies a less conservative approach to the selection of assessment factors based on an overview of the data for the whole group. From the available toxicity data, it is clear that fish and invertebrates (Daphnia) are more sensitive than algae to this type of substance, so it is assumed in all assessments for which there are no algal data that this would not give a lower NOEC value than those from fish or Daphnia. This then allows an assessment factor of 10 to be used when only NOECs for fish and Daphnia are available. This applies to tert-butylphenyldiphenyl phosphate, 2-ethylhexyldiphenyl phosphate, tricresyl phosphate, isopropylphenyldiphenyl phosphate (and tris(isopropylphenyl) phosphate), and isodecyldiphenyl phosphate. Any further testing on these substances is unlikely to result in a higher aquatic PNEC.

For tetraphenyl resorcinol diphosphate, the PNEC is derived from only one NOEC, but as an assessment factor of 10 is used on this single value, further testing would not lead to a higher PNEC value.

For triphenyl phosphate, the PNEC is derived from the two available NOEC values with an assessment factor of 50. A long-term invertebrate test could result in an increased PNEC; the predicted Daphnia NOEC would suggest a possible four-fold increase which would not change the conclusions significantly.

For the other substances (cresyl diphenyl phosphate and trixylenyl phosphate), predicted values are used as there are no (or insufficient) measured toxicity data. These values could be revised through (additional) testing; depending on the accuracy of the predictions, the resulting PNECs could be higher or lower.

Overall, additional aquatic toxicity testing would make little difference to the conclusions.

## 4.3 Further information on toxicity to sediment organisms

Almost all the assessments have PEC/PNEC ratios greater than one for sediment for some scenarios. Therefore further information on the toxicity to sediment organisms would be useful to refine the PNECs for this endpoint.

If the aquatic compartment as a whole (sediment and surface water) is considered, the most useful information will probably be obtained by testing substances that have a log  $K_{ow}$  above five. For substances with a log  $K_{ow}$  below five, the risk characterisation for the sediment compartment is identical to that of the surface water compartment (since the equilibrium partitioning approach is used); although sediment toxicity testing may remove the concern for the sediment compartment for these substances, there might still be a concern for surface water.

The situation is different for the substances with a log  $K_{ow}$  above five in that the resulting PEC/PNEC ratios are increased by a factor of 10 to take account of direct ingestion of sediment-bound substance. In this case, any refinement of the assessment for the surface water compartment will not necessarily be reflected in the assessment of the sediment compartment.

Methods for using sediment toxicity test data outlined in the TGD mean that there is little to be gained from carrying out a single long-term test, unless it is known that the species tested is sensitive to this type of substance.

#### 4.4 Further information on toxicity to soil organisms

Several of the assessments have PEC/PNEC ratios greater than one for soil. The PNECs for this endpoint are based on the equilibrium partitioning approach, and the PEC/PNEC ratios have again been increased by a factor of 10 for substances with log  $K_{ow}$  above five to take into account the possibility of direct ingestion of soil-bound substance. Further information on the toxicity to soil organisms would be useful to refine the PNECs for this endpoint.

Methods for using soil toxicity test data outlined in the TGD mean that there is little to be gained from carrying out a single long-term test, unless it is known that the species tested is sensitive to this type of substance.

### 4.5 Further information on degradation and distribution in the environment

The degradation rates used in the assessment are mainly based on default values from the TGD for readily or inherently biodegradable substances supported by the available data from simulation studies. However, for some substances for which it is not possible to refine the PEC or PNEC by other means, it may be useful to carry out a soil degradation simulation study from which a reliable half-life for degradation in the soil compartment can be derived. This would allow PECs for the soil compartment to be refined (with implications for the PECs for secondary poisoning via the earthworm food chain and human exposure via the environment).

Further information on the actual rates of degradation in the environment in surface water and especially sediment would also, in principle, be useful for the assessments of those substances considered to be inherently biodegradable. Information on degradation in soil would be useful in those cases where a risk is identified for the regional soil compartment. A representative degradation half-life is needed in any case for the two substances considered to meet the screening PBT criteria.

A further area for consideration is the fate of substances in waste water treatment plant (WWTP). The SimpleTreat program in EUSES was used to estimate the fate and distribution of substances in this assessment, and this depended on both the default biodegradation rate and the estimated  $K_{oc}$ . Direct measurements on the amounts removed in sludge and released to water could be used in place of the calculated values. These would need to include measurements at representative sites and include public WWTP receiving industrial effluent as well as industrial WWTP.

Related to the above point, the adsorption potential of most of the substances (represented by the  $K_{oc}$ ) is estimated, and this has a significant influence on its predicted partitioning behaviour in the environment. There is some evidence for triphenyl phosphate that the prediction method might underestimate the  $K_{oc}$  for this type of substance. A sensitivity analysis has been performed in Annex D, and this shows that a higher  $K_{oc}$  value would affect the conclusions, but not necessarily in a straightforward (or especially significant) way. Further testing for sediment sorption coefficient is suggested for triphenyl phosphate, and this could indicate a need for further studies with the other substances.

## 4.6 Further evaluation of the available avian and mammalian toxicity data

As noted in the individual assessments, there are limited data on avian and mammalian toxicity suitable to derive PNECs for secondary poisoning and to assess risks from human exposure through the environment. Further literature searches or the provision of test reports might allow some changes to be made. Specific questions or issues related to individual studies are included in the individual risk evaluation reports. Table 3.6 indicates those endpoints for which data are currently insufficient for classification, and further information on some of these (in particular the repeated-dose and reproductive/developmental toxicity) would be of use in the assessments of secondary poisoning and humans exposed through the environment. For trixylenyl phosphate and tris(isopropylphenyl) phosphate, there are no suitable data from which to develop a PNEC for secondary poisoning, and for these two plus isopropylphenyl diphenyl phosphate and tertbutylphenyl diphenyl phosphate, the data do not allow an assessment of human exposure through the environment.

#### 4.7 Summary

In principle, a great deal more information is needed to refine the aryl phosphate assessments. However, it should be possible to read across information obtained for one substance to other substances using similar methods to those already employed in

the assessments. This would apply to both exposure and effects information. On this basis, the following strategy is suggested for filling the data gaps:

- Collect any further information on emissions to the environment, especially from processing steps and from losses over the service life of treated articles. This could include measurements of levels in WWTP effluent and sludge, as well as information on emission control measures.
- In parallel, further long-term testing of sediment and soil organisms for selected substances should be considered. It is suggested that triphenyl phosphate, an isopropylated phenyl phosphate (preferably with a high proportion of isopropylated phenyl groups), either 2-ethylhexyl diphenyl phosphate or isodecyl diphenyl phosphate, and tetraphenyl resorcinol diphosphate be considered. These cover the different structural types present in the group (the unsubstituted phenyl, alkyl-substituted phenyl, alkyl diaryl and diphosphate types). An alternative approach to substance selection is considered below.

#### The normal test species are:

- · Lumbriculus (sediment);
- Chironomus (sediment);
- Hyallela (sediment);
- higher plants (soil) (a plant test is already available for isopropylated triphenyl phosphate);
- earthworms (soil);
- nitrification inhibition (soil).

The need for further information for these and other aryl phosphates should be reconsidered once the results of the initial substances are available. The use of three species each for sediment and soil should allow the most suitable test, in terms of sensitivity, to be identified and so any further testing that might be needed for other substances can then be suitably targeted. It may also be possible to develop relationships between the effect concentrations and properties of the substances which would allow the toxicity of other aryl phosphates to be predicted. The need for any further degradation testing should also be considered at this stage.

For comparison, the possible testing requirements for each substance under the REACH legislation are set out in Appendix 1 of this summary.

#### Alternative approach to substance selection

The selection of substances for testing is based on the different chemical structures present in the group being assessed. This assumes that variation in toxicity is related to the structure. An alternative approach to selection would be to test substances at the ends of the toxicity range (or the ranges of other properties). This would then allow predictions for other substances to be interpolated between the available data and avoid extrapolations. The main problem with this approach is that there is currently no clear indication of what property or properties are related to toxicity –  $\log K_{ow}$  is often used in such relationships but did not show a strong relationship for these assessments (see Annex B).

Looking at the PNECs for the aquatic compartment (recognising that many of these are based on predicted values), tricresyl phosphate has the lowest (most toxic) value, tetraphenyl resorcinol diphosphate has the highest PNEC, and triphenyl phosphate is towards the middle of the range. Looking at the calculated PNECs for sediment, where

the sorption also has an influence, tricresyl phosphate still has the lowest value, and tetraphenyl resorcinol diphenyl phosphate is the second highest (2-ethylhexyl diphenyl phosphate has the highest value). Of the other substances selected on the basis of structure, isodecyl diphenyl phosphate has the second lowest PNEC, and tris(isopropylphenyl) phosphate is the third highest. The positions based on the soil PNEC are the same as for sediment. Hence an alternative selection to take account of the spread of toxicity values could replace triphenyl phosphate with tricresyl phosphate, and prefer isodecyl diphenyl phosphate over 2-ethylhexyl diphenyl phosphate. The selection would therefore be: tricresyl phosphate, an isopropylated phenyl phosphate with a high proportion of isopropylated phenyl groups, isodecyl diphenyl phosphate and tetraphenyl resorcinol diphosphate.

# 5 New information being generated under the US HPV Programme

A number of substances have had test plans developed as part of the US High Production Volume (HPV) Programme. A summary of the tests being carried out, and the preliminary results so far obtained, are shown in Table 5.1, along with the possible significance for the risk assessment.

Table 5.1 Summary of new information generated under the US HPV programme

Substance	Property	Preliminary result	Comment
Tertbutyl diphenyl phosphate	Boiling point	Above 400°C	Final result published. Information already incorporated into the assessment
	Vapour pressure	1.08×10 <sup>-3</sup> Pa at 20°C	Final result published. Information already incorporated into the assessment.
	Log K <sub>ow</sub>	4.85	Final result published. Information already incorporated into the assessment.
	Hydrolysis	Hydrolyses at pH 5, 7 and 9.	Final result published. Information already incorporated into the assessment.
Trixylenyl phosphate	Water solubility	0.0186 mg/l at 25°C	Value is lower than assumed in assessment.
	Photo- degradation	Determined the UV-visible absorption below pH 2, around pH 7 and above pH 10.	Data are difficult to use directly in the assessment.
	Hydrolysis	No degradation at pH 4 in preliminary study. Definitive study gives half-lives (at 25°C) of over a year at pH 7 and 219 days at pH 9.	The degradation pattern seen is similar to that already described in the assessment.
	Bio- degradation	OECD 301D – not readily biodegradable.	Similar to results already included in the assessment.
	Fugacity modelling	Not yet available.	Modelling has already been carried out in the assessment.
	Acute toxicity to fish	Fathead minnows: 96-hour LC <sub>50</sub> above 1.12 mg/l (measured concentration).	Similar to results already included in the assessment that show no effects at solubility. Does not affect PNEC.
	Acute toxicity to Daphnia	48-hour EC <sub>50</sub> = $0.06$ mg/l (measured concentration).	No data currently available. Does not affect PNEC but would lead to a change in the classification proposal from R51/53 to R50/53.
	Toxicity to algae	96-hour EC <sub>50</sub> above 1.01 mg/l, 96-hour NOEC = 0.11 mg/l (based on initial measured conc.). Endpoint was biomass.	Does not affect the PNEC.

Substance	Property	Preliminary result	Comment
Tetraphenyl resorcinol	Boiling point	Above 400°C	Consistent with value used in risk assessment.
diphosphate	Vapour pressure	2.59×10 <sup>-3</sup> Pa at 20°C	Value is higher than used in assessment. The value appears to be out of line for the information available for aryl phosphates as a whole.
	Log K <sub>ow</sub>	4.93	Value is slightly lower, but similar to, the value used in the assessment.
	Water solubility	1.05 at 20°C	Value is slightly higher, but similar to, the value used in the assessment.
	Photodegra dation estimate	Absorption coefficients were obtained at acid, neutral and basic pH.	Data are difficult to use directly in the assessment.
	Fugacity modelling	Not yet available.	Modelling has already been carried out in the assessment.

## Appendix 1 - Possible testing requirements under REACH

This appendix considers the possible testing requirements for environmental endpoints only.

The tables in this appendix show the data availability for each of the aryl phosphates in relation to REACH Regulation (Annexes VII to X). The resulting testing requirements are listed underneath each table. These assume no read-across between members of the group of aryl phosphates assessed in this series of reports (that is, the methods derived in Annex B are not used, and no assumptions are made based on the overall data set, such as "algal NOECs are always higher than fish or invertebrates"). Some QSAR predictions are included and have been taken as being sufficient for the purposes of REACH – these are methods which were developed "externally" and not for the purpose of the assessment. An example is that used for predicting hydrolysis rates for some substances.

Decisions on testing for the later annexes (Annex IX and X) are based on conclusions in the risk evaluation reports. It is clear that the exposure assessments could be revised (and presumably the exposure scenarios developed in the suppliers' Chemical Safety Assessments (CSAs) will be different, to take account of these conclusions), and this would or could have an impact on what further testing is needed (this has not been taken into account in this appendix). For most substances, the use pattern is quite complex and so simple comments on the effect of refined exposure data cannot be made. However, risk characterisation ratios for cresyl diphenyl phosphate are only a little above one, and so only a relatively small reduction in emissions would be needed to remove the risks for all compartments. Also, trixylenyl phosphate has a limited use pattern and should be amenable to a relatively straightforward revision of the exposure assessment.

The testing requirements under REACH are driven by the tonnage initially and then by the results of the Chemical Safety Assessment. For the purpose of this exercise, the substances are all assumed to fall into the highest tonnage band (above 1,000 tonnes per year).

Where long-term terrestrial testing is indicated, this includes the microorganism test included in Annex IX.

Under biodegradation, Annex IX indicates that simulation testing is not needed if the substance is readily biodegradable. This has been followed in the tables below. However, adjustment to the half-life in soil due to sorption means that the half-lives for readily biodegradable substances which have high sorption can be lengthy. In such cases, a measured half-life in soil might affect the calculated local concentrations, and so simulation testing could be considered as an additional test.

#### Triphenyl phosphate

Annex	Endpoint	Remarks
Annex VII	Short-term invertebrate Algal Ready biodegradability	Available. Available. Data available to allow identification as readily biodegradable.
Annex VIII	Short-term fish Activated sludge inhibition Hydrolysis Adsorption/desorption screening	Available. Suitable alternative data. Available. Data available might be considered not clear.
Annex IX*	Long-term invertebrate Long-term fish Simulation testing (water, soil, sediment)	No results available. Available. Not needed, as substance is readily biodegradable. However, further testing to investigate the actual degradation (mineralization) half-life in sediment and soil under relevant environmental conditions might have an impact on the assessment.
	Bioaccumulation in fish Further sorption/desorption	Available. May be of use in view of currently available data.
	Short-term terrestrial effects	No data. CSA has risks to terrestrial compartment from equilibrium partition. High sorption measured, and indicated by log K <sub>ow</sub> , so long-term testing indicated (plus microorganisms test from this annex).
Annex X*	Further biodegradation (not specified)	Nothing indicated.
	Further environmental fate (not specified)	Nothing indicated.
	Long-term terrestrial effects Long-term sediment effects Long-term/repro birds	No data. CSA has risks so testing indicated. No data. CSA has risks so testing indicated. No avian data. PNEC derived from mammalian data considered reliable, so no testing.
Notes:	* Need for these largely dependent	testing. t on the CSA results

Notes:

- Further sorption/desorption studies
- Long-term Daphnia test.
- Possible further study of sorption/desorption.
- Long-term terrestrial testing.
- · Long-term sediment testing.

<sup>\*</sup> Need for these largely dependent on the CSA results.

#### Tertbutylphenyl diphenyl phosphate

Annex	Endpoint	Remarks
Annex VII	Short-term invertebrate Algal Ready biodegradability	Available.  No data (no details available so marked as 4.)  Data available to allow identification as readily biodegradable.
Annex VIII	Short-term fish Activated sludge inhibition Hydrolysis	Available No data available. No data, estimation based on appropriate QSAR.
	Adsorption/desorption screening	No data, estimation from log K <sub>ow</sub> . Testing indicated as degradation not rapid on timescale of sorption.
Annex IX*	Long-term invertebrate Long-term fish Simulation testing (water, soil, sediment)	Available. Available. Not needed, as substance readily biodegradable. However, further testing to investigate the actual degradation (mineralization) half-life in sediment and soil under relevant environmental conditions might have an impact on the assessment.
	Bioaccumulation in fish Further sorption/desorption	Available.  May be needed depending on outcome of screening test.
	Short-term terrestrial effects	No data. Risks indicated in CSA, so testing should follow. High log K <sub>ow</sub> value indicates high sorption, extra factor of 10 used, so long-term testing probably indicated (would need the microorganisms test in any case).
Annex X*	Further biodegradation (not specified)	Nothing indicated.
	Further environmental fate (not specified)	Nothing indicated.
	Long-term terrestrial effects Long-term sediment effects Long-term/repro birds	No data. CSA has risks so testing indicated. No data. CSA has risks so testing indicated. No avian data. PNEC derived from mammalian data considered reliable, so no testing.
Notes:	* Need for these largely dependent	

- Algal test.
- Activated sludge inhibition test.
- Sorption/desorption screening, possible further testing to follow.
- Long-term terrestrial testing (from next level but indicated due to high sorption, unless this is contradicted by the sorption testing).

#### Isopropylated triphenyl phosphate

The assessment considers the data on substances with different degrees of alkylation where these can be distinguished. The overall conclusion is that for aquatic effects there is no clear difference across the range and so they are considered to have the same values. In the table below, the aquatic effects data are considered to apply to all. This could be the basis for a category approach for these substances, for their aquatic effects at least.

Annex	Endpoint	Remarks
Annex VII	Short-term invertebrate Algal Ready biodegradability	Available. Not certain, one water-accommodated fraction study with no details, others invalid. Data available to show IPPDPP is readily biodegradable; TIPPP considered inherently
Annex VIII	Short-term fish Activated sludge inhibition Hydrolysis	biodegradable. Available. Available. No data, estimation based on appropriate QSAR.
	Adsorption/desorption screening	No data, estimation from log K <sub>ow</sub> . Testing indicated as degradation not rapid on timescale of sorption.
Annex IX*	Long-term invertebrate Long-term fish Simulation testing (water, soil, sediment)	Available. Available. Testing indicated for TIPPP for PBT assessment (IPPDPP is readily biodegradable).
	Bioaccumulation in fish	Available for IPPDPP, not for TIPPP. Testing indicated for TIPPP.
	Further sorption/desorption	May be needed depending on outcome of screening test.
	Short-term terrestrial effects	No data. Risks indicated, so testing should follow. High log K <sub>ow</sub> value indicates high sorption, extra factor of 10 used, so long-term testing probably needed (would need the microorganism test in any case).
Annex X*	Further biodegradation (not specified)	Simulation testing for TIPPP would exhaust possibilities.
	Further environmental fate (not specified)	An earthworm BCF test could be performed if terrestrial food chain risks were still predicted.
	Long-term terrestrial effects	Plant test available. Further testing indicated by CSA, as equilibrium partition gives lower result.
	Long-term sediment effects Long-term/repro birds	No data. Testing indicated by CSA. PNEC for IPPDPP based on avian data, no testing indicated. Not possible to derive a PNEC for TIPPP, so avian testing possibly indicated.

Notes:

<sup>\*</sup> Need for these largely dependent on the CSA results.

- Algal study.
- Sorption/desorption screening, possible further testing to follow.
- Simulation testing for TIPPP.
- Bioconcentration in fish for TIPPP.
- Long-term terrestrial testing.
- Long-term sediment testing.
- (Avian testing for TIPPP).
- Possibly an earthworm BCF test.

#### Trixylenyl phosphate

Annex	Endpoint	Remarks
Annex VII	Short-term invertebrate	No data (possible result from US HPV programme mentioned but no details).
	Algal	Available.
	Ready biodegradability	Sufficient data to conclude that inherently degradable.
Annex VIII	Short-term fish	Available
	Activated sludge inhibition	Suitable alternative data.
	Hydrolysis	No data, estimation based on appropriate QSAR.
	Adsorption/desorption screening	No data, estimation from log $K_{\text{ow}}$ . Testing indicated as degradation not rapid on timescale of sorption.
Annex IX*	Long-term invertebrate	No data. CSA has risks so testing indicated.
	Long-term fish	No data. CSA has risks so testing indicated.
	Simulation testing (water, soil, sediment)	Required as half-life needs to be established for PBT assessment.
	Bioaccumulation in fish	Available.
	Further sorption/desorption	May be needed depending on outcome of screening test.
	Short-term terrestrial effects	No data. Risks indicated in CSA, so testing should follow. High log K <sub>ow</sub> value indicates high sorption, extra factor of 10 used, so long-term testing probably indicated (would need the microorganisms test in any case).
Annex X*	Further biodegradation (not specified)	Simulation testing would exhaust possibilities.
	Further environmental fate (not specified)	Nothing indicated.
	Long-term terrestrial effects	No data. CSA has risks so testing indicated.
	Long-term sediment effects	No data. CSA has risks so testing indicated.
	Long-term/repro birds	No suitable data for secondary poisoning
	3 3 3 3 3 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4	PNEC. Avian testing indicated in absence of mammalian data.

Notes: \* Need for these largely dependent on the CSA results.

The limited use pattern means that refining the exposure assessment should be possible.

- Sorption/desorption screening, possible further testing to follow.
- Long-term invertebrate test (no need for short-term test if this done).
- · Long-term fish test.
- Simulation testing for degradation.
- Long-term terrestrial testing.
- Long-term sediment testing.
- (Avian testing).

#### Tetraphenyl resorcinol diphosphate

Annex	Endpoint	Remarks
Annex VII	Short-term invertebrate Algal Ready biodegradability	Available. Available. Data available to conclude that inherently biodegradable.
Annex VIII	Short-term fish Activated sludge inhibition Hydrolysis Adsorption/desorption screening	WAF test only. Suitable alternative data. Available. No data, estimation from log K <sub>ow</sub> . Testing indicated as degradation not rapid on timescale of sorption.
Annex IX*	Long-term invertebrate Long-term fish Simulation testing (water, soil, sediment) Bioaccumulation in fish	Available, with reservations.  No data.  Could be considered as substance is inherently biodegradable.  No data. Estimation possible, but testing indicated.
	Further sorption/desorption Short-term terrestrial effects	May be needed depending on outcome of screening test.  No data. Risks indicated in CSA, so testing should follow. High log K <sub>ow</sub> value indicates high sorption, extra factor of 10 used, so long-term testing probably indicated (would need the microorganisms test in any case).
Annex X*	Further biodegradation (not specified) Further environmental fate (not specified)	Nothing indicated.
	specified) Long-term terrestrial effects Long-term sediment effects Long-term/repro birds	No data. CSA has risks so testing indicated. No data. CSA has risks so testing indicated. No avian data. PNEC derived from mammalian data considered reliable, so no testing.

Notes:

- Sorption/desorption screening, possible further testing to follow.
- Long-term fish test (so short-term test not needed).
- Simulation testing for degradation.
- Bioaccumulation test.
- Long-term terrestrial testing.
- Long-term sediment testing.

<sup>\*</sup> Need for these largely dependent on the CSA results

#### 2-Ethylhexyl diphenyl phthalate

Annex	Endpoint	Remarks
Annex VII	Short-term invertebrate Algal	Available. Available study not assignable, so possible gap.
	Ready biodegradability	Available.
Annex VIII	Short-term fish Activated sludge inhibition Hydrolysis Adsorption/desorption screening	All available studies not assignable. Available. No data. Specific predictions not made. Available study not useable. Estimate used.
Annex IX*	Long-term invertebrate Long-term fish Simulation testing (water, soil, sediment)	Available. Available study not assignable. Not needed, as substance readily biodegradable. However, further testing to investigate the actual degradation (mineralization) half-life in sediment and soil under relevant environmental conditions mighave an impact on the assessment.
	Bioaccumulation in fish Further sorption/desorption Short-term terrestrial effects	Available.  May be needed to confirm estimate.  No data. Risks indicated in CSA, so testing should follow. High log K <sub>ow</sub> value indicates high sorption, extra factor of 10 used, so long term testing probably indicated (would need the microorganisms test in any case).
Annex X*	Further biodegradation (not specified)	Nothing indicated.
	Further environmental fate (not specified)	An earthworm BCF test and studies on plant uptake from soil could be performed if terrestrial food chain risks were still predicted
	Long-term terrestrial effects Long-term sediment effects Long-term/repro birds	No data. CSA has risks so testing indicated. No data. CSA has risks so testing indicated. No avian data. PNEC derived from mammalian data considered reliable, so no testing.

Notes:

- Algal test.
- Hydrolysis.
- Sorption/desorption screening, possible further testing to follow.
- Long-term fish test (so short-term test not needed).
- Long-term terrestrial testing.
- Long-term sediment testing.
- Possibly an earthworm BCF test and plant uptake study.

<sup>\*</sup> Need for these largely dependent on the CSA results.

#### Isodecyl diphenyl phosphate

Annex	Endpoint	Remarks
Annex VII	Short-term invertebrate Algal Ready biodegradability	Available. Available. Data available to allow identification as inherently biodegradable.
Annex VIII	Short-term fish Activated sludge inhibition Hydrolysis Adsorption/desorption screening	Available. Suitable alternative data. No data. Specific predictions not made. No data, estimation from log K <sub>ow</sub> . Testing indicated as degradation not rapid on timescale of sorption.
Annex IX*	Long-term invertebrate Long-term fish Simulation testing (water, soil, sediment) Bioaccumulation in fish Further sorption/desorption Short-term terrestrial effects	Available. Available. Could be considered as substance is inherently biodegradable. Available. May be needed depending on outcome of screening test. No data. Risks indicated in CSA, so testing should follow. High log K <sub>ow</sub> value indicates high sorption, extra factor of 10 used, so long-term testing probably indicated (would need the microorganisms test in any case).
Annex X*	Further biodegradation (not specified)	Nothing indicated.
	Further environmental fate (not specified)	An earthworm BCF test and studies on plant uptake from soil could be performed if terrestrial food chain risks were still predicted
	Long-term terrestrial effects Long-term sediment effects Long-term/repro birds	No data. CSA has risks so testing indicated. No data. CSA has risks so testing indicated. No avian data. PNEC derived from mammalian data considered reliable.
Notes:	* Need for these largely dependent	on the CSA results

- Hydrolysis.
- Sorption/desorption screening, possible further testing to follow.
- Simulation testing for degradation.
- Long-term terrestrial testing.
- · Long-term sediment testing.
- Possibly an earthworm BCF test and plant uptake study.

#### Cresyl diphenyl phosphate

Annex	Endpoint	Remarks
Annex VII	Short-term invertebrate Algal Ready biodegradability	Available. Available. Data available to show substance is readily biodegradable.
Annex VIII	Short-term fish Activated sludge inhibition Hydrolysis Adsorption/desorption screening	Available. Available. Available. No data, estimation from log K <sub>ow</sub> . Testing indicated as degradation not rapid on timescale of sorption.
Annex IX*	Long-term invertebrate Long-term fish	Available.  No data. PNEC based only on measured values would lead to risks (although less than estimated PNEC), so CSA indicates need for testing.
	Simulation testing (water, soil, sediment) Bioaccumulation in fish Further sorption/desorption	Not needed, as substance is readily biodegradable. Available. May be needed depending on outcome of
	Short-term terrestrial effects	screening test.  No data. Risks indicated in CSA (although only a few scenarios and low ratios), so testing should follow. High log K <sub>ow</sub> value indicates high sorption, so long-term testing probably indicated (would need the microorganisms test in any case).
Annex X*	Further biodegradation (not specified)	Nothing indicated here.
	Further environmental fate (not specified)	Nothing indicated here.
	Long-term terrestrial effects	No data. CSA has limited risks so testing indicated.
	Long-term sediment effects	No data. CSA has limited risks so testing indicated.
	Long-term/repro birds	Available; PNEC based on mammalian data

For this substance, only a small reduction in emissions would be needed to remove the risks for all compartments.

- Sorption/desorption screening, possible further testing to follow.
- Long-term fish test.
- Long-term terrestrial testing.
- Long-term sediment testing.

#### Tricresyl phosphate

Endpoint	Remarks
Short-term invertebrate Algal Ready biodegradability	Available. Available. Data available to allow identification as readily biodegradable.
Short-term fish Activated sludge inhibition Hydrolysis Adsorption/desorption screening	Available. Available. Available. Limited data, estimation from log K <sub>ow</sub> . Testing indicated as degradation not rapid on timescale of sorption.
Long-term invertebrate Long-term fish Simulation testing (water, soil, sediment) Bioaccumulation in fish Further sorption/desorption Short-term terrestrial effects	Available. Available. Not indicated as needed, as substance is readily biodegradable. Available. May be needed depending on outcome of screening test. No data. Risks indicated in CSA, so testing should follow. High log K <sub>ow</sub> value indicates high sorption, extra factor of 10 used, so long-term testing probably indicated (would need the microorganisms test in any case).
Further biodegradation (not specified)	Nothing indicated here.
	Nothing indicated here.
Long-term terrestrial effects Long-term sediment effects	No data. CSA has risks so testing indicated. No data. CSA has risks so testing indicated.
	Short-term invertebrate Algal Ready biodegradability  Short-term fish Activated sludge inhibition Hydrolysis Adsorption/desorption screening  Long-term invertebrate Long-term fish Simulation testing (water, soil, sediment) Bioaccumulation in fish Further sorption/desorption  Short-term terrestrial effects  Further biodegradation (not specified) Further environmental fate (not specified)

Notes:

- Sorption/desorption screening, possible further testing to follow.
- Long-term sediment testing.
- Long-term terrestrial testing.

Need for these largely dependent on the CSA results.

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