

Decabromodiphenyl Ether Flame Retardant in Plastic Pallets

A Safer Alternatives Assessment

Appendices

Prepared for:

Maine Department of Environmental Protection

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Appendix 1

Distributors of Plastic Pallets

Company Name	Address
<u>Name</u>	<u>Location</u>
Akro-Mils	<u>Akron, Ohio United States</u>
Albion Industries	<u>Albion, Michigan United States</u>
B & R Unifuse	<u>Staatsburg, New York United States</u>
<u>Cadillac Industrial Products Co.</u>	<u>Troy, Michigan United States</u>
Cartonplast LLC	<u>De Forest, Wisconsin United States</u>
Casemaker <u>Inc.</u>	<u>Thornhill, ON Canada</u>
Colson Caster Corp.	<u>Jonesboro, Arkansas United States</u>
Convoy, Inc.	<u>Canton, Ohio United States</u>
Cookson Plastic Molding	<u>Latham, New York United States</u>
Creative Techniques, Inc.	<u>Auburn Hills, Michigan United States</u>
DIC Intl. USA Inc.	<u>Ft. Lee, New Jersey United States</u>
Dynaric, Inc.	<u>Virginia Beach, Virginia United States</u>
EAM Mosca Corp.	<u>West Hazleton, Pennsylvania United States</u>
Faultless Caster	<u>Evansville, Indiana United States</u>
FKI Logistex Automation Div.	<u>Cincinnati, Ohio United States</u>
Flexcon Container	<u>Springfield, New Jersey United States</u>
Frost Inc.	<u>Grand Rapids, Michigan United States</u>
General Container Corp.	<u>Somerset, New Jersey United States</u>

Globe Composite Solutions	Rockland, <u>Massachusetts United States</u>
Goodwrappers	Baltimore, <u>Maryland United States</u>
Gould Plastics, Inc.	Duluth, <u>Georgia United States</u>
<u>Hoover Materials Handling Group, Inc.</u>	Alpharetta, <u>Georgia United States</u>
Intech Corp.	Closter, <u>New Jersey United States</u>
Interroll Corp.	Wilmington, <u>North Carolina United States</u>
IPL Products, Ltd.	Worcester, <u>Massachusetts United States</u>
Jarvis Caster Group	Palmer, <u>Massachusetts United States</u>
JECO Plastic Products, LLC	Plainfield, <u>Indiana United States</u>
Kornylak Corp.	Hamilton, <u>Ohio United States</u>
Linpac Materials Handling	Georgetown, <u>Kentucky United States</u>
LINPAC Materials Handling	<u>Georgetown, Kentucky USA</u>
Lyon Workspace Products	Aurora, <u>Illinois United States</u>
Macro Plastics, Inc.	Fairfield, <u>California United States</u>
Melmat Inc.	Huntington Bch., <u>California United States</u>
<u>Mid-States Engrg. & Mfg., Inc.</u>	<u>Milton, Iowa United States</u>
Molded Fiber Glass Tray Co.	Linesville, <u>Pennsylvania United States</u>
Molded Materials Inc.	Plymouth, <u>Michigan United States</u>
Ohio Rack, Inc.	Alliance, <u>Ohio United States</u>
OptiLogistics, Inc.	Irving, <u>Texas United States</u>
Pacific Bin Corp.	Bellevue, <u>Washington United States</u>
PDQ Plastics, Inc.	Bayonne, <u>New Jersey United States</u>
Plastic Products, Inc.	Schaumburg, <u>Illinois United States</u>
Port Erie Plastics	Harborcreek, <u>Pennsylvania United</u>

	<u>States</u>
Protecta-Pack Systems	Minneapolis, <u>Minnesota United States</u>
Quantum Storage Systems	Opa-Locka, <u>Florida United States</u>
Rampmaster Inc.	Miami, <u>Florida United States</u>
Regplas, Inc.	Mission, <u>Kansas United States</u>
Remcon Plastics, Inc.	Reading, <u>Pennsylvania United States</u>
SCA Packaging North America	New Brighton, <u>Pennsylvania United States</u>
Sealed Air Corp.	Danbury, <u>Connecticut United States</u>
Sealed Air Corp.	Saddle Brook, <u>New Jersey United States</u>
SFB Plastics, Inc.	Wichita, <u>Kansas United States</u>
Shuert Industries Inc.	Sterling Hts., <u>Michigan United States</u>
Signode Packaging Systems	Glenview, <u>Illinois United States</u>
SJF Material Handling Inc.	Winsted, <u>Minnesota United States</u>
SKF USA	Bethlehem, <u>Pennsylvania United States</u>
Smith Companies, Inc.	Pelham, <u>Alabama United States</u>
Sol Plastics. <u>L.P.</u>	<u>Montreal, QC Canada</u>
Superior Tire & Rubber Co.	Warren, <u>Pennsylvania United States</u>
Tente Casters, Inc.	Hebron, <u>Kentucky United States</u>
Timco Inc.	Peekskill, <u>New York United States</u>
Tote Systems Inc.	Burleson, <u>Texas United States</u>
Transpac Corp.	Lansing, <u>Michigan United States</u>
UFP Technologies Inc.	Georgetown, <u>Massachusetts United States</u>
Vestil Mfg. Co.	Angola, <u>Indiana United States</u>

Appendix II

Grocery Industry Pallet Performance Specifications¹

- 1) Exact 48-inch x 40-inch dimensions. Square in each direction.
- 2) True four-way entry. Capable of accommodating existing pallet jacks from all four sides (as opposed to current style with cutouts and stringers).
- 3) Minimum-width pallet jack openings of 12 inches and minimum height of **3- 3/4** inch clearance when under load. Width of each center support must be less than six inches to accommodate pallet jacks.
- 4) Smooth, non-skid, top-bearing surface should have at least 85% coverage. However, 100% is preferred. Non-skid surface should be flat, or have no indentations or protrusions that could cause product damage.
- 5) Bottom-bearing surface of no less than 60% coverage with properly placed cut-outs (12-inches square) for pallet jack wheels from four sides. Surface should be flat or have no indentations or protrusions that could cause product damage.
- 6) All bottom entry edges should be chamfered to 1/4-inch for easy entry and exit.
- 7) Overall height of platform should not exceed six inches.
- 8) Rackable from both the 48-inch and 40-inch dimensions. Allowable deflection in drive-in and drive-through racks no more than 1/2 inch.
- 9) Compatible with pallet conveyors, pallet dispensers, skate-wheel pallet-flow racks, and automatic storage and retrieval systems.
- 10) No protruding fasteners.

¹ Grocery Manufacturers of America, Grocery Industry Pallet Subcommittee (written by Cleveland Associates), "Recommendations on the Grocery Industry Pallet System," p.11.

- 11) Must be made of material that does not contaminate the product it carries.
- 12) Must meet or exceed current pallet resistance to fire.
- 13) Must be recyclable. Preferably made from recycled material.
- 14) Desired weight under 50 pounds.
- 15) Load capacities of 2,800 pounds. Capable of bearing 2,800-pound loads safely in stacks five loads high.
- 16) Repairs should be economically feasible.
- 17) Weather resistant.
- 18) Moisture resistant.
- 19) Capable of safely moving product, damage free, through the entire distribution channel with multiple cycles (from manufacturer through distributor to retail).

Appendix III

Idle Material Handling Products (FM Approval Class Number 4996)



The storage of idle material handling products in warehouses or manufacturing facilities can represent a severe challenge to automatic sprinkler protection systems. Products such as pallets, tote boxes, bins or protective cases, especially when manufactured from plastic, wood or cellulosic materials, normally require a very high sprinkler water discharge rate for adequate protection.

While doing extensive research testing, FM Approvals has developed a system and a test methodology to determine if the tested material can be protected as equivalent to wood pallets.

All FM Approved material handling products have been tested according to FM Approvals Standard 4996, "The Classification of Idle Plastic Pallets as Equivalent to Wood Pallets." The Approvals standard specifically addresses idle plastic pallets.

For specific sprinkler protection recommendations, refer to FM Global Property Loss Prevention Data Sheet 8-9, "Storage of Class 1, 2, 3, 4 and Plastic Commodities" and FM Global Property Loss Prevention Data Sheet 8-24, "Idle Pallet Storage."

Approval recognition is extended only to those products which exhibit burning and heat release characteristics equivalent to or less critical than conventional wood pallets. Each FM Approved product shall bear an Approval mark.

...

Plastic Pallets (Class Number 4996)



Group Products by Company

CHEP International Inc
8517 South Park Circle, Orlando, Florida 32819, USA

Product	Listing Country	Certification Type
P4840B	United States of America	FM Approved
B4840A	United States of	FM

Product	Listing Country	Certification Type
	America	Approved

iGPS Company LLC
225 East Robinson St, Suite 200, Orlando, Florida 32801, USA

Product	Listing Country	Certification Type
BiPP4840 HR 6R iGPS Pool Pallet	United States of America	FM Approved

Orbis Corporation
1055 Corporate Center Dr, Oconomowoc, Wisconsin 53066-0389, USA

Product	Listing Country	Certification Type
Model 1200x1000 (39x47) FM SuperPal	United States of America	FM Approved
Model 36 x 42 FM FG	United States of America	FM Approved
Model 36 x 48 FM FG	United States of America	FM Approved
Model 40 x 48 FM BulkPal	United States of America	FM Approved
Model 40 x 48 FM HDSC	United States of America	FM Approved
Model 40 x 48 FM RACK'R	United States of America	FM Approved
Model 40 x 48 FM RCKO	United States of	FM

Product	Listing Country	Certification Type
	America	Approved
Model 40 x 48 FM RCKO LP	United States of America	FM Approved
Model 40 x 48 OP FM CIISF	United States of America	FM Approved
Model 40 x 48 OP FM CIISF LP	United States of America	FM Approved
Model 40x48 Stack'R Pallet	United States of America	FM Approved
Model 42 x 48 FM HDSC	United States of America	FM Approved
Model 44 x 56 DC HI	United States of America	FM Approved
Model 44 x 56 DC LO	United States of America	FM Approved
Model 44 x 56 OCP	United States of America	FM Approved
Model 45 x 48 FM HD Lip A	United States of America	FM Approved
Model 45 x 48 FM HD Lip B	United States of America	FM Approved
Model 45 x 48 FM HD Lip C	United States of America	FM Approved
Model 45 x 48 FM JOURNEY	United States of America	FM Approved
Model 48 x 48 FM Drum OP CIISF	United States of America	FM Approved

Product	Listing Country	Certification Type
Model 48 x 48 FM HD DRM	United States of America	FM Approved
Model 48 x 48 FM HDSC	United States of America	FM Approved
Models 40 x 48 FM GrabPal 2.5",3.7," GrabPal 3.0" con	United States of America	FM Approved

Plastics Research Corporation
1400 South Campus Ave, Ontario, California 91761-4330, USA

P/N 105250-101 is a high performance composite pallet designed to comply with GMA requirements for a 40 x 48 in (1 x 1.2 m), 4-way, rackable, non-reinforced pallet, capable of multi-trip duty. This pallet does not contain decca-bromine.

Product	Listing Country	Certification Type
P/N 105250-101 Plastic Pallet	United States of America	FM Approved

Polymer Solutions International
15 Newtown Wood Road, Newtown Square, Pennsylvania 08055, USA

Product	Listing Country	Certification Type
4048 Prostack general purpose plastic pallets	United States of America	FM Approved
4048 Prostack with Lip general purpose plastic pallets	United States of America	FM Approved
4048 Prostack with Cleat and Corner Openings plastic pallets	United States of America	FM Approved

Schoeller Arca Systems Inc
3000 Town Center, Suite 620, Southfield, Michigan 48075, USA

Product	Listing Country	Certification Type
BiPP4840 HR 6R iGPS	United States of America	FM Approved

TMF Corporation
850 West Chester Pike, Suite #303, Havertown, Pennsylvania 19083-4439, USA

Product	Listing Country	Certification Type
Model Protech 4048	United States of America	FM Approved

Appendix IV: UL 2335 Classified Pallets



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POLYMER PALLETS L L C	Pallets, Storage	QENL.R19299
REHRIG PACIFIC CO	Pallets, Storage	QENL.R20575
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QENL.R25484

Pallets, Storage

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CHEP EQUIPMENT POOLING SYSTEMS

R25484

8517 S PARK CIR

ORLANDO, FL 32819 USA

Pallet Name	General Description	Pallet Length (inches)	Pallet Width (inches)
P4840B - V2.0	Four-Way Entry, Block Pallet	48	40

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POLYMER PALLETS L L C

R19299

U S 422

15567 MAIN MARKET RD

PO BOX 674

PARKMAN, OH 44080 USA

Pallet Name	General Description	Pallet Length (inches)	Pallet Width (inches)
Polymer Pallet	PVC Two-Way Entry, Stringer Pallet	48	48
Polymer Pallet	PVC Two-Way Entry, Stringer Pallet	48	42
Polymer Pallet	PVC Two-Way Entry, Stringer Pallet	42	48

Polymer Pallet	PVC Two-Way Entry, Stringer Pallet	44	44
Polymer Pallet	PVC Two-Way Entry, Stringer Pallet	48	40
Polymer Pallet	PVC Two-Way Entry, Stringer Pallet	40	48
Polymer Pallet	PVC Two-Way Entry, Stringer Pallet	42	42
Polymer Pallet	PVC Two-Way Entry, Stringer Pallet	36	48
Polymer Pallet	PVC Two-Way Entry, Stringer Pallet	40	40
Polymer Pallet	PVC Two-Way Entry, Stringer Pallet	36	36
Polymer Pallet	PVC Four-Way Entry, Block Pallet	48	48
Polymer Pallet	PVC Four-Way Entry, Block Pallet	48	42
Polymer Pallet	PVC Four-Way Entry, Block Pallet	42	48
Polymer Pallet	PVC Four-Way Entry, Block Pallet	44	44
Polymer Pallet	PVC Four-Way Entry, Block Pallet	48	40
Polymer Pallet	PVC Four-Way Entry, Block Pallet	40	48
Polymer Pallet	PVC Four-Way Entry, Block Pallet	42	42
Polymer Pallet	PVC Four-Way Entry, Block Pallet	36	48
Polymer Pallet	PVC Four-Way Entry, Block Pallet	40	40
Polymer Pallet	PVC Four-Way Entry, Block Pallet	36	36

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REHRIG PACIFIC CO

R20575

4010 E 26TH ST

LOS ANGELES, CA 90023 USA

Pallet Name	General Description	Pallet Length (inches)	Pallet Width (inches)
HuskyLite Snap-Lock Pallet	Four-Way Entry, Block Pallet	48	40
HuskyLite Snap-Lock Pallet	Four-Way Entry, Block Pallet	48	36
HuskyLite Snap-Lock Pallet	Four-Way Entry, Block Pallet	43	37
HuskyLite Snap-Lock	Four-Way Entry, Block	41.3	37.4

Pallet	Pallet		
HuskyLite Snap-Lock Pallet	Four-Way Entry, Block Pallet	37	37

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SCHOELLER ARCA SYSTEMS INC

R25482

SUITE 110

5202 OLD ORCHARD RD

SKOKIE, IL 60077 USA

Pallet Name	General Description	Pallet Length (inches)	Pallet Width (inches)
BiPP 4840 HR 6R iGPS PoolPallet-SAS	Four-Way Entry, Block Pallet	48	40

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Appendix V

Polymer Range for Flame Retardant Plastic Pallets

Prepared for this report by:
James Innes & Ann Innes
Flame Retardants Associates

The polymer resins most likely to be chosen by a formulator for the flame retardant plastic pallet application include the polyolefins (PP, PE) and/or MPPO. The polyolefin resins are from a technical perspective the easiest to flame retard while retaining the physical properties required for a plastic pallet AND doing so at the least cost to produce.

Further, after significant review of flame retardant plastic pallet technology and marketplace, it is apparent to the authors that only two specific polyolefin polymer resins will practically fit the flame retardant plastic pallet application. These are HDPE, high density polyethylene, and polypropylene copolymer or impact modified polypropylene. The process for making the pallet is injection molding (although there are some thermoformers). The pallet making process largely governs the selection of melt flow of the chosen polymer. The polymer must be able to be injection molded in such a process; i.e., melt flow appropriate for the process. Either virgin resin or post-industrial recycle resin would be chosen. Of importance to note is that HDPE is the resin found in most post-consumer PE as it is used in the overly- abundant milk containers sold across the country. This is a blow molding grade and is not applicable to injection molding. The table below is an abbreviated list of polypropylene and HDPE suppliers, trade names and grades of HDPE that could fit the flame retardant plastic pallet application.

HDPE Suppliers, Trade Names, HDPE Grades

Suppliers	Trade Names	Grades/Comments
Chevron Phillips	Marlex HWN4550 HDPE 5 MFI*	Tensile Strength 3500 ⁺ psi Flex Modulus 160-180 (10 ³ psi ASTM D790) Izod Impact 6 ⁺ fl lb/in (Notched)
Equistar Chemicals LP	Alathion M4661 HDPE 6 MFI	
Exxon Mobil	Escorene HD 6705 HDPE Escorene HD 0358 HDP	
Ineos	Fortilene KG4685 PP	
Phillips Sumika	Marlex AGN120	
Equistar Chemicals	Petrothene PP38NR01X01	
Lyondell Basell	Moplen EP340M	

*MFI = Melt Flow Index

In the 1990's GE Plastics, now SABIC, developed several new applications for their Noryl® polymer. This included a "plastic house" and they did also develop a plastic pallet which actually

went through the requisite pallet testing at FM to prove the formulation met the FM standard for idle pallets. Noryl® is modified polyphenylene oxide (or ether) blended with high impact polystyrene or HIPS. The amount of HIPS in the formulation depends on the flow needed for the application. In addition to these two polymers, the formulations also include 10-15% of a phosphate ester plasticizer which results in a UL94 V0 formulation. [A lower loading (~6-8%) of the phosphate ester would likely result in a pass in the idle pallet test; however, physical properties would require consideration.] Various plasticizers have been used since the initial development. Most recently, these have been alkylated phenol phosphate or bisphenol A diphosphate. The pallet produced was deemed to be too expensive to market and, as a result, GE did not renew the certification with FM and did no further development. Flame Retardants Associates estimates that a pallet produced with Noryl® which meets the pallet standards would be in the economically prohibitive range of over \$90/pallet. Also, there is little or no post-industrial MPPO available in the recycle marketplace which could result in lower cost.

Appendix VI

The Cost Factor and Flame Retardant Plastic Pallets

Prepared for this report by:
James Innes & Ann Innes
Flame Retardants Associates

Specific gravity is an important concept to understand. Why? Because it directly impacts the cost factor for producing a pallet. Indeed, it is the controlling part of the cost factor. Specific gravity can be defined as the density (mass per unit volume) of any material divided by that of water at a standard temperature (usually 4°C). Since water's density is nearly 1.00 g/cc, density in g/cc and specific gravity are nearly equal.

What does this mean? For a given volume of material, a plastic compound with a lower specific gravity will produce a part with lower weight. Or it actually takes less pounds of material to fill a mold to produce the part. A given amount of a plastic compound or formulation with a lower specific gravity will produce more parts than another formulation with a relatively higher specific gravity. Molds are filled on a volume basis, not weight. One of the resulting "tricks of the trade" is knowing that a less costly formulation which meets all the part's requirements across the board may simply not be economically attractive if its specific gravity is too high. In other words, needing more of the compound to fill the mold often wipes out the advantage of the lesser cost per pound.

From this point forward, a review of formulation costs incorporating the absolutely required specific gravity factor will be presented. This should help the reader understand how to do the cost calculation as well as the direct impact on cost of specific gravity.

If a 40" x 48" rackable standard pallet weighs 44.2 pounds using a non-flame retardant PP resin, flame retardant (FR) versions will produce pallets weighing amounts different than that. See Table App-VI-1 for the calculations which incorporate specific gravity data. These calculations assume a 0.9 specific gravity for the PP resin and a 0.95 specific gravity for the DECA/antimony trioxide FR system, and 1.048 for the MDH FR system.

Table App-VI-1. Calculating the Weight of FR Plastic Pallets

PP Pallet (no FR) Weight	Weight of Pallet with Deca/Antimony as FR	Weight of Pallet with MDH as FR
44.2 pounds	$44.2/0.9 \times 0.95^1 = 46.65$ pounds	$44.2/0.9 \times 1.048 = 51.46$ pounds

¹ Let's assume a 50 pound pallet which contains 3.4 pounds of DECA and 1.133 pounds of antimony trioxide (this is a 3 to 1 ratio). A formulator would probably do a calculation using an even 100 pounds. So the calculation of the 0.95 specific gravity for the DECA/antimony/PP system is obtained as follows:

90.934 pounds PP sp grav of 0.9 $0.90934/0.9 = 1.0103$ cc (cubic centimeters)

6.8 pounds DECA sp grav 3.25 $0.068/3.25 = 0.0292$ cc

2.266 pounds antimony trioxide sp grav 5.6 $0.02266/5.6 = \underline{0.0040}$ cc

Total cc = 1.0435 cc

Or for the DECA FR system $1/1.0435 = 0.95$ sp gravity

The iGPS Pallet

Now, as an example, let's look at some hypothetical calculations for the iGPS FR pallet, starting with specific gravity.. This pallet is made from HDPE, not PP, and is flame retarded with a DECA/antimony trioxide system. It contains about 3.4 pounds DECA and is expected to contain 1.133 pounds antimony trioxide using a 3 to 1 ratio (which is typical for this system). Let's convert this 48.5 pound pallet to a formulation batch weighing 100 pounds to make the calculations easier.

3.4 pounds DECA/ 48.5 pounds pallet mass = 7.01% loading (let's round that to 7.0)

1.133 pounds antimony trioxide/48.5 pounds pallet mass = 2.37% loading

We have 7 pounds of DECA + 2.37 pounds of antimony trioxide = 9.37 pounds. So in a 100 lbs batch, that means we have 90.63 pounds of HDPE (or this is a 90.63% loading).

We know the specific gravity of HDPE ranges from 0.952 to 0.965, so let's use 0.96 for our calculation here.

0.9063 HDPE/ 0.96 sp grav = 0.9440

0.070 DECA/ 3.25 sp grav = 0.0215

0.0237 Sb₂O₃/ 5.6 sp grav = 0.0042

Total = 0.9697 cc/gram

$1/0.9697 = \mathbf{1.0312}$ specific gravity for this DECA/Antimony HDPE formulation. This is the density of this formulation in grams per cc.

Now let's move on to some cost calculations for this iGPS DECA FR HDPE pallet.

A simple calculation of total formulation raw material cost per pound using the raw material component costs would be done as shown in Table 14. In this table, the colorants/stabilizer cost/pound was gathered from current commercial stabilizer/colorant suppliers.

Table App-VI-2. Simple DECA FR HDPE formulation cost calculation

Formulation Component	Loading	Cost/pound	Component Cost
HDPE	88.63%	\$0.80	\$0.709
DECA	7.0%	\$1.80	\$0.126
Antimony Trioxide (Sb ₂ O ₃)	2.37%	\$3.00	\$0.0711
Colorants/Stabilizers	2%	\$2.50	\$0.05
Formulation Total Cost/pound			\$0.9561

But the reality of actually trying to produce a formulation like this and push it into an injection molding machine to produce a large part like a pallet means that in all likelihood a masterbatch would be used. This masterbatch (think concentrate) is let down in the pallet injection molding machine at a loading level that produces the required amount of FR system in the formulation being injected into the pallet mold. A masterbatch is produced by a masterbatch compounder. See Figure App-VI-1 for a list of known commercial suppliers of masterbatch compound. Each has supplied a full range of masterbatch needed for plastic pallet manufacture.

Masterbatch Supplier	Location
Spartech Polycom	Denora, PA
Washington Penn Plastics	Washington, PA
PolyOne Corporation	Avon Lake, OH
Phoenix Plastics	Conroe, TX
Saco Polymers (formerly Padanaplast)	Aurora, OH
Hanson Company	Duluth, GA

Figure App-VI-1. Commercial Masterbatch Suppliers

A typical masterbatch would contain 60% active FR in a HDPE. See Table App-VI-3 for the masterbatch cost calculation.

Table App-VI-3. DECA/Antimony Trioxide HDPE Masterbatch Cost Calculation

Formulation Component	Loading	Cost/pound	Component Cost
HDPE	40%	\$0.80	\$0.32
DECA	44.82%	\$1.80	\$0.806
Antimony Trioxide (Sb ₂ O ₃)	15.18%	\$3.00	\$0.455
Formulation Total Cost/pound			\$1.581

The cost calculation for this masterbatch plus the cost to compound plus a markup for profit gives a good estimate of the sell price per pound of this masterbatch to the pallet molder. In this case, let's assume \$0.20/pound as a cost of compounding which gives a cost of \$1.781/pound for the masterbatch producer to produce this formulation. The masterbatch producer will mark this up to make a profit so let's assume a 30% markup. This produces a cost per pound to the pallet injection molder of \$2.54. Now let's use this cost and recalculate in Table App-VI-4 the raw material cost for the iGPS FR pallet (in other words, we are now re-doing the calculation costs in Table App-VI-2 to reflect real world use of masterbatch). To provide the required 7% DECA in 100 pounds of the final compound, 15.61 pounds of the \$2.54/pound masterbatch will be required. ($7\% / 44.82\% = 15.6\%$)

Table App-VI-4. Pallet Formulation Cost Calculation Using Deca FR Masterbatch

Formulation Component	Loading	Cost/pound	Component Cost
HDPE	82.39%	\$0.80	\$0.659
DECA Masterbatch	15.6%	\$2.54	\$0.396
Colorants/Stabilizers	2%	\$2.50	\$0.05
Formulation Total Cost/pound			\$1.105

So a better estimate of the raw material cost per pound for the Deca FR pallet is \$1.105 rather than the \$0.9561 computed in Table App-VI-2.

More Costs – Plastic Resins and Plastic Pallets

The cost of producing a flame retardant plastic pallet varies significantly depending on the base resin and the chosen flame retardant. Table App-VI-5 shows price ranges for three of the more likely resins for the FR plastic pallet application. [Plastics News, 9/27/10, pp. 21-22]

Table App-VI-5. Price Ranges for Likely Plastic Pallet Resins

Resin	Grade/Description	Price range/pound
HDPE	Injection Molding	\$0.80-\$0.85
	Recycle	\$0.41-\$0.45
PP	Injection General Purpose	\$0.97-\$1.03
	Large Buyers*	\$0.66 - \$0.67
	Recycle Industrial	\$0.62-\$0.68
PPO/PPE	Injection General Purpose	\$1.23-\$1.87

*London Metals Exchange for very large buyers, Plastics News, Sept 6, 2010

Cost to purchase pallets in the pallet industry today ranges from \$5 per pallet for a wood pallet to \$60 per pallet for a 50 pound plastic (non-FR) pallet to a halogen FR pallet at about \$100 per pallet which weigh about 55 pounds.

Plastic Pallet using a Metal Hydrate FR system

Now let's look at the cost to produce a plastic pallet using PP and a MDH (magnesium hydroxide) non-halogen flame retardant. Since we now live in the real world, we need to calculate a masterbatch cost first. See Table App-VI-6.

Table App-VI-6. Cost Calculation for non-halogen FR Masterbatch

Formulation Component	Loading	Cost/pound	Component Cost
PP	28%	\$1.00	\$0.28
MDH	70%	\$0.35	\$0.245
Processing Aid	2%	\$1.20	\$0.024
Formulation Total Cost/pound			\$0.549

Adding a \$0.20 cost to compound gives a cost to manufacture of \$0.749 per pound. Add a 30% markup for a price to the pallet molder of \$1.07 per pound.

To provide 23% MDH in the final compound, 40 pounds of masterbatch will be used. So now we can compute the cost of raw materials. See Table App-VI-7.

Table App-VI-7. Raw Material Cost for a MDH FR PP Pallet using a PP FR Masterbatch

Formulation Component	Loading	Cost/pound	Component Cost
PP	58%	\$1.00	\$0.58
MDH-PP Masterbatch	40%	\$1.07	\$0.428
Black Masterbatch	1%	\$2.00	\$0.02
UV Thermal Concentrate	1%	\$3.00	\$0.03
Formulation Total Raw Material Cost/pound			\$1.058

Let's look at specific gravity calculations for this non-halogen FR PP approach.

For the masterbatch, we have (let's leave out the process aid for this calculation):

PP at 0.28/0.9 sp grav = 0.3111 cc and MDH at 0.70/2.36 sp grav = 0.2966 cc for a total of 0.6077 cc/gram or 1.6455 grams per cc.

For the final MDH FR PP, we have:

PP at 0.58/0.9 sp grav = 0.6444
 MDH Masterbatch at 0.4/1.6455 = 0.2431
 Additives at 0.02/0.9 = 0.0222
 Total = 0.9097 or 1/0.9097 = 1.0993 grams/cc (sp gravity)

So for a comparison, the density of the DECA containing iGPS HDPE pallet was 1.0312 while the density for our MDH FR PP pallet is 1.0993. So if iGPS or anyone else were to make a FR plastic pallet from our MDH FR PP formulation, the weight of that pallet in the same mold used for the iGPS pallet would be calculated as follows:

48.5 pounds x 1.0993/1.0312 = 51.7 pounds

Therefore, the non-halogen FR PP pallet made in the iGPS mold goes a little over the 50 pound mark (which is the recommended upper weight limit by the GMA).

What about using a phosphorus FR system in a plastic pallet?

The use of phosphorus flame retardants such as APP, APP derived compounds, and EDAP have not really found application in non-halogen FR plastic pallets, or many other applications for that matter. This is likely mostly due to first the fact that halogen FR's continue to be used and are cost/performance effective and secondly to a perception that phosphorus FR systems are just too costly. However, they may very well be worth taking a look at in a plastic pallet application since the flammability requirement, "burn like wood", is far lower than a more stringent requirement to be self-extinguishing. So let's take a look at the cost situation for EDAP as an example.

The cost for a typical FR PP formulation using EDAP , such as Unitex FR44-94S, that is expected to meet idle pallet requirements (this formulation has not been tested in this type of test as far as the authors know) would be calculated as in Table App-VI-8.

Table App-VI-8. Cost Calculation for an FR PP Formulation using EDAP

Formulation Component	Loading	Cost/pound	Component Cost
PP	86%	\$1.00	\$0.86
EDAP	12%	\$2.50	\$0.30
Stabilizers	2%	\$2.50	\$0.05
Formulation Total Raw Material Cost/pound			\$1.21

With the \$0.20/pound compounding cost and 30% profit, we have a cost to the pallet producer of \$2.01/pound.

Specific gravity of EDAP is 1.3. The formulation specific gravity is:

$$\text{PP at } 0.86/0.9 \text{ sp grav} = 0.9555$$

$$\text{EDAP at } 0.12/1.3 = 0.0923$$

$$\text{Additives at } 0.02/0.9 = \underline{0.0222}$$

$$\text{Total} = 1.07 \text{ or } 1/1.07 = 0.9346 \text{ grams/cc (sp gravity)}$$

A disadvantage of this system is that the EDAP compound cannot be introduced using a masterbatch but must instead be added during the compounding operation. (A second heat history is not a good thing when it comes to phosphorus compounds.) Recall that for the DECA and metal hydrate FR systems, a masterbatch can be used.

The same formulation might also work with HDPE as the resin. In such a case, the specific gravity of the formulation would be:

HDPE at 0.86/0.96 sp grav	= 0.8958
EDAP at 0.12/1.3	= 0.0923
Additives at 0.02/0.9	= <u>0.0222</u>
Total	= 1.0103 or 1/1.0103 = 0.99 grams/cc (sp gravity)

So what does all of this mean? It means that since the iGPS pallet weighs about 48.5 pounds and has a specific gravity of 1.0312 (see highlighted result on p. 24 above), then this HDPE-EDAP formulation with a specific gravity of 0.99 would produce a pallet that weighs 46.6 pounds. (48.5/1.0312 x 0.99)

The net result then is the iGPS pallet made using the DECA masterbatch would cost 48.5 pounds of material times the HDPE-DECA cost of \$1.105/pound or \$53.59. Whereas the HDPE-EDAP formula pallet weighs 46.6 pounds with a cost of material to the pallet producer of \$2.01/pound or a price of \$93.66. So herein lays the drawback to the phosphorus approach. The final cost is prohibitively high – at least in comparison to other options. The same problem occurs when considering APP with a specific gravity of 1.8 and a HDPE-APP formulation cost equivalent to the HDPE-EDAP cost of \$2.01/pound. The pallet weight is slightly higher at about 47.8 pounds and the cost is still above \$90 per pallet.

So in summary it seems logical to conclude that a non-halogen FR plastic pallet is going to have to start with a metal hydrate, probably magnesium hydroxide, and a polyolefin resin, probably PP. ATH could be used as well but temperatures must be kept low and so the resin with this FR must be HDPE (as PP is processed above the ATH water release temperature). Polypropylene is a little more costly on \$/pound purchase price than HDPE, but hopefully we have now learned that the initial cost per pound has nothing to do with the cost of the material going into the mold. The cost and specific gravity calculations must be performed first to get a true picture of the cost to fill the pallet mold.

The exact formulation components and cost numbers in the real world will be different than those shown here because we have simplified the formulations to make it easier to understand the calculation principles and because prices fluctuate on a daily basis for almost all materials. The important thing to learn is that there is a lot involved in developing a balanced formulation. When flame retardants are loaded into formulations, especially those needing to meet more stringent flammability standards (more stringent than “burn like wood”), the physical property most impacted is tensile strength. The tensile strength goes down and translated to a pallet in use, this means it will be more likely to break under load. However, at the reduced FR loadings needed for a FR plastic pallet, the adverse impact on tensile strength as well as other properties is lessened considerably. (This helps support the argument that making a non-halogen FR plastic pallet is feasible.)

Appendix VII: Innovative and Novel Non-Halogen Flame Retardants

Nicholas A. Zaksek, Manager of Applications Research and Development, JJI Technologies
[Paper presented at ANTEC 2010 by David Diefenthal and sponsored by Society of Plastic Engineers]

Abstract

JJI Technologies bases its technology platform on developing innovative and novel non-halogen flame retardants and plastic additives. Our self-catalyzed technology embedded within the flame retardant enhances physical performance, increases extinguishing efficiency, and simplifies the compounding process. Our JJAZZ™ FR boasts features such as low smoke and odor when exposed to flame. This is achieved by forming a robust char barrier that stops the flame from propagating to the polyolefin. Features such as a low specific gravity, lower loading levels, and non-blooming help to exemplify the overall cost savings and improved aesthetics that benefit the user.

Introduction

The demands for flame retarded materials continues to increase with building material and electrical component markets pushing toward the use of polymers in increasing numbers of end applications. There are 3 basic constituents that must be considered when flame retarding polymers; the effectiveness of the flame retardant, the physical properties, and the sustainability of the product throughout its life cycle.

In most applications, the additions of non-halogen flame retardants are considered to be fillers as opposed to an additive. This is especially true in the case of metal hydroxides and hydrates where the loadings comprise of more than fifty percent of the polymer system. The addition of filler to a polymer often dramatically impacts the physical properties of the polymer. The effectiveness of the flame retardants to reduce flame spread, smoke generation, and in many cases extinguish the flame establishes its value in the market. The necessary loading of the flame retardant to meet the demands of stringent flame tests, also effects the latter. Finally, sustainability has become a rapidly increasing concern among plastic compound manufacturers as well as flame retardant producers. Regulations are driving initiatives to recycle and preserve the environment. The importance of “green” products has become more prevalent than ever before.

Flame retardants can no longer maintain a pristine image by proving safe in their usable form. They are scrutinized from the point of manufacturer, how safe they are for exposure to humans and pets, what by-products occur when they burn (i.e. toxic smoke, carcinogens), and their end of life. Bioaccumulation, decomposition products, heavy metals, small molecules, halogens, PBB and PBDE's, and recyclability are all concerns that the new generations of flame retardants have

to answer too.¹ This paper serves to illustrate that through innovative knowledge and technology; JJI Technologies is developing and improving its flame retardant additives to meet the demands of the market and its customers.

JJAZZ Physical Properties

JJAZZ™ is a free flowing white powder available in three particle sizes to meet physical and dielectric application demands (Figure 1, 2). The powder is a neutral pH and exhibits a low specific gravity to reduce compound weight. With the lower loading levels needed to flame retard a compound, it is easy to color. The aesthetics of products are also enhanced since the JJAZZ™ does not exhibit any surface migration. All of the properties contribute to an efficient flame retardant that is non-toxic, generates less smoke, and is fully recyclable. A chart illustrates a full comparison of JJAZZ™ as well as other products JJI currently has in development (Figure 3).

Results and Discussion

Upon investigating traditional non-halogen flame retardants, metal hydroxide and hydrate flame retardants are limited due to the excessively high loading necessary to achieve acceptable performance results. These excessively high loadings significantly impact physical properties as well as adding weight to the final compound.² Intumescent flame retardants, like those in the ammonium polyphosphate family, allow loading levels to be reduced, thus preserving the properties of the base resin. Unfortunately, most of these flame retardants need a synergist, usually a pentaerythritol, which needs to be added congruently for the system to be fast-acting and completely effective. This synergist has proven to be the Achilles heel of these FR's due to it being hydrolytically weak coupled with the inability to insure full dispersion (Figure 4).³

Mechanisms

The reason for the addition of a synergist lies in the mechanism of how intumescent systems work. They are comprised of three components: an acid source (APP), a carbon source (pentaerythritol), and a blowing agent (typically melamine) which all need to interact with each other in a prescribed sequence of events^{4,5}. The acid source breaks down to dehydrate the carbon source. Once this process is complete; the blowing agent has to decompose in order to form a protective heat sink char⁶.

JJAZZ™ not only utilizes the above method of action, but also reacts to form nitrogen gas to dilute the fuel source and prevent the acid source from volatilizing away before it can react with the carbon source.

Char Formation

JJAZZ™ has overcome the hurdles noted above by embedding a proprietary catalyst to eliminate the need for the addition of a synergist. This self catalyzing technology ensures good distribution at a molecular level (Figure 5). This allows for superior distribution and functionality

within the polymer which decreases loading levels. Also this would improve the physical properties of the final product. The technology also serves two additional purposes; it creates low activation energy and a fast deploying char. JJAZZ™ also creates a dual layer char consisting of initially a hard and glassy char, accompanied by a porous and highly insulating char upon continued exposure to flame. This unique mechanism may require additional additives in a standard FR system. This is clearly illustrated by the two maximum decomposition point shown by TGA analysis (Figure 6).

JJAZZ™ Performance Data

All performance data will vary due to resin selection, the final application, and the additives package that is utilized in the compound. Several addition levels of JJAZZ™ were compounded on a 50mm twin screw extruder in a 7 melt flow rate polypropylene to illustrate the minimal impact JJAZZ addition has on the final compound. These loading levels are in accordance with tests that require more stringent and rigorous burn testing requirements. One additional note is that the melt flow rate was measured at a lower temperature in order to keep the FR from prematurely activating. The data is listed in a chart below (Figure 7).

Processing Parameters

JJAZZ™, like other phosphorous based FR's, does have processing limitations and is therefore limited to polyolefins and some rubber compounds. Typical processing temperatures on an extrusion unit should not exceed 390°F (~200°C). JJI Technologies provides support on proper extrusion parameters in order to achieve the optimal compound results (Figure 8, 9).

Continued R&D

It has been noted that not one flame retardant can fill every need. The key to success of the application is optimizing intumescent systems to react as near to the base resin decomposition point as possible. Various temperature ranges, as well as decomposition behavior of plastics and test methods dramatically affects how readily a compound can be flame retarded. This requires flame retardants to offer a variety of temperature ranges as well as extinguishing mechanisms to meet every market demand. JJI Technologies has a committed R&D effort to span this gap and diversify its product lines to not just meet, but exceed these demands (Figure 10). There is also an ongoing effort within JJI Technologies to innovate current technologies to enhance the robustness of our JJAZZ™ processing by increasing the temperature stability.

Figure 1. Dielectric properties of 2.5 μm

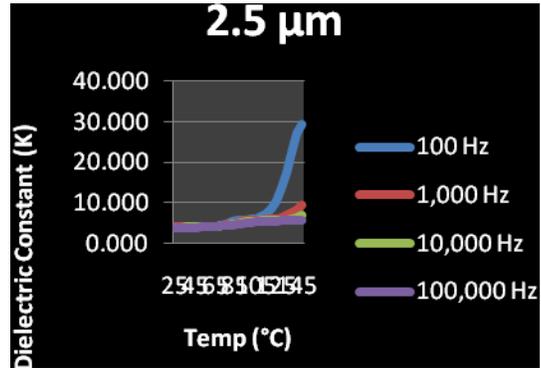


Figure 2. Dielectric properties of 6 μm

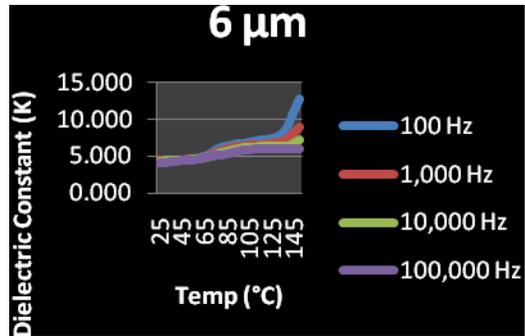


Figure 3. JJI product properties

Physical Property	JJAZZ®	*DP-110
Appearance	White Powder	White Powder
Decomposition Temp (2%, Nitrogen)	>230°C (464°F)	N/A
Activation Temp	~250°C (482°F)	~345°C (653°F)
Bulk Density	400	400
Phosphorus Content	15-17%	N/A
Nitrogen Content	>20%	N/A
pH	7.2	7.2
Specific Gravity	1.30	1.28

*DP-110 is in development

Figure 4. Conventional 2 component technology

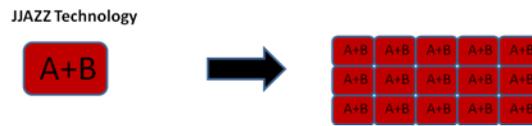


*Gray indicates inactive

*An X indicates hydrolytically compromised

*Red and blue indicate active sites

Figure 5. JJAZZ™ single component technology



*All pairs are active

Figure 6. TGA and DSC analysis of char mechanism

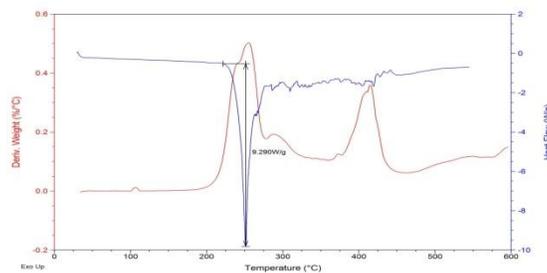


Figure 7. Performance Data

	Control	31% JJAZZ™	35% JJAZZ™	40% JJAZZ™
UL 94 1.6mm	Fail	V2	V0	V0
Specific Gravity	0.901	1.04	1.02	1.03
Hardness (Shore A)	87.5	81.8	84.5	86.5
MFI	3.72	1.53	1.55	0.98
Notch Izod	7.857	1.243	1.101	1.079
Tensile at Break	2536	1906	1789	1709
Elongation at Break	51.21	66.61	51.52	30.72
Flex Modulus	173205	202987	217319	245448

Units

- MFI (melt flow index) – (190°C/2.16kg)
 - Notch Izod – (ft-lb/in)
 - Tensile – (psi)
 - Elongation – (%)
 - Flex Modulus – (psi)

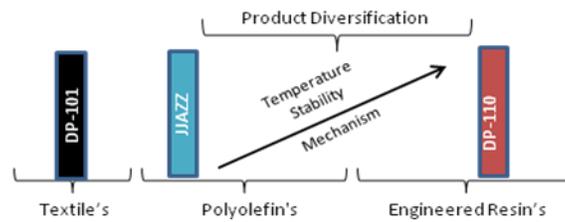
Figure 8. JIAZZ™ Processing Parameters

Die	Zone 5	Zone 4	Zone 3	Zone 2	Zone 1
380	370	340	340	350	350

Figure 9. Suggested extruder set-up

- 11 barrel extruder
 - Ambient vent at barrel 6
 - Side feeder at barrel 7
 - Vacuum at barrel 10
 - Pellet and powder in barrel 1
- A 1:2 feed ratio of powder from the rear feeder to the side feeder

Figure 10. Product Diversification



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Appendix VIII: Plastics Flammability Tests: Smaller Scale Laboratory Tests

Prepared for this report by:
James Innes & Ann Innes
Flame Retardants Associates

UL 2335 and FM 4996 are the only tests for determining whether a flame retardant polymer pallet meets NFPA 13 requirements. But other tests are sometimes mentioned in the context of flame retardant plastics. Discussed below are smaller scale lab tests that often come up in discussion of fire resistant pallet testing. Some are actually more useful than others with regard to non-halogen fire resistant plastic pallets.

Testing with the Fire Propagation Apparatus

After a pallet has passed the FM 4996 test, any subsequent resin or formulation changes must be evaluated using the Fire Propagation Apparatus. If the results from this test are inconclusive, then full scale testing under the FM 4996 standard must be performed again. The Fire Propagation Apparatus is a piloted ignition open air test protocol using two 4 inch x 4 inch plaques or sheets of pallet material placed one on top of the other. The sample is exposed to external heat flux values up to 60 kW/m². Time to ignition is recorded along with other ignition-related data. To determine fire properties, the sample is exposed to radiant heat flux of 50 kW/m². Fire properties such as chemical heat release rate, mass loss rate, CO generation, and optical density of smoke are measured. This data is then used to judge if a formulation change must undergo the more costly full scale FM 4996 test protocol.

OI or LOI (Limiting Oxygen Index)

The OI or LOI test is a simple, small-scale test whose technical requirements are specified in ASTM D2863. This test measures the minimum amount of oxygen needed to support the burning process. The test is conducted in an oxygen/nitrogen atmosphere on 3 test specimens (6.5 mm wide strips of plastic) in a way that mimics candle-like burning conditions. Numerical results indicate the percentage of oxygen required to support burning of the sample. For example, a result of 28 means 28% of

the oxygen/nitrogen atmosphere was oxygen and this was the amount required to just support the burning process. (Oxygen is required for burning to take place. See FR101 in the next section.) Our atmosphere on planet Earth contains about 21% oxygen. So a result in the test of 28 indicates a good degree of flame retardancy. Theoretically, such a test specimen would resist burning in a real fire scenario as atmospheric oxygen does not reach a level of 28%. See Figure App-VIII-1 for the LOI test apparatus. [“Plastic Flame Retardants: Technology and Current Developments,” J. Innes & A. Innes, Rapra Review Reports, 2003. P. 7]

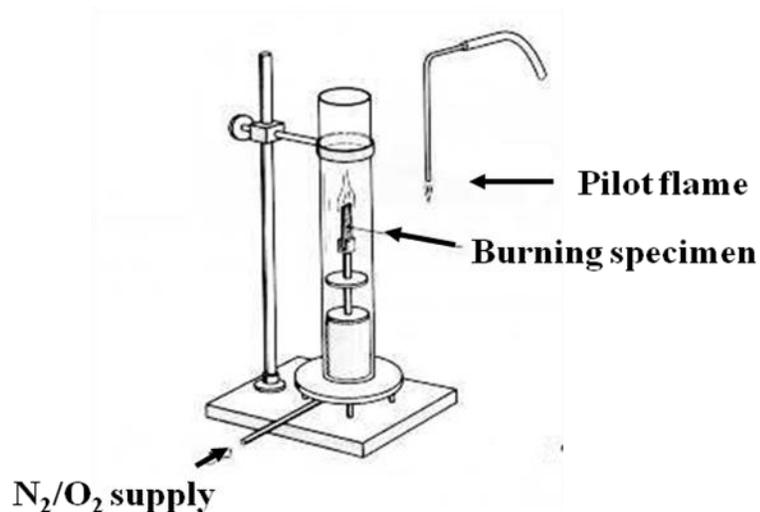


Figure App-VIII-1. LOI Test Apparatus

UL94 (Underwriters Laboratories)(Harmonized with ISO 9772, 9773)

Underwriters Laboratories UL94 test, Test for Flammability of Plastic Materials for parts in Devices and Appliances or Standard for Safety of Flammability of Plastic Materials for Parts in Devices and Appliances Testing, is perhaps the most well known flame retardant (FR) test in the industry. It has been and still is widely used for a variety of plastic materials which end up in an even wider variety of applications. This test together with UL746 A-C tests form the basis for the recognition of plastics as summarized in UL’s Recognized Components Directory. UL94 applies to electrical parts, appliances, consumer and office equipment as well as other application areas *except* the use of

plastics in buildings. [“Plastics Flammability Handbook,” Jurgen Troitzsch, Carl Hanser Verlag, 2004, p. 533]. The UL94 standard actually contains several test protocols. The most common involves a vertical burn method and bar-shaped test specimens (13 mm x 125 mm of varying thicknesses such as 1/8”, 1/16”, 1/32”). The test bar is suspended a specified distance above a lump of cotton while a calibrated burner flame is applied to the specimen for 10 seconds, burn time of the specimen after removal of the flame is recorded, then the flame is applied to the specimen a second time for 10 seconds, and the burn time is again recorded. This procedure is followed for a set of five test bars. Performance in the test is indicated by burn time (usually in seconds) for each specimen, total after-flame burn time for all specimens, afterglow time, and the existence of flaming drips which may ignite the cotton. See Figure App-VIII-2 for the UL94 test apparatus sketch and Table App-VIII-1 for the UL94 test classification criteria. The result is actually expressed in this protocol as UL94 V0, V1, or V1 plus the thickness of the tested specimen. [“Plastic Flame Retardants,” Innes & Innes, p. 7.]

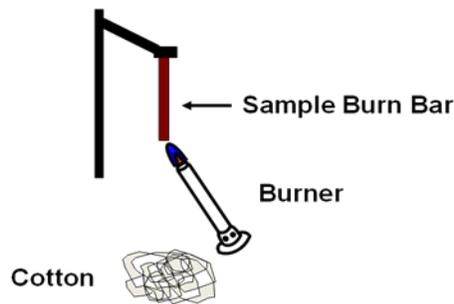


Figure App-VIII-2. UL 94 Test Apparatus

Table App-VIII-1. UL94 Materials classification (vertical burn test procedure)

Criteria	UL94 V0	UL94 V1	UL94 V2
Afterflame time for each individual specimen t_1 or t_2	≤ 10 s	≤ 30 s	≤ 30 s
Total afterflame ($t_1 + t_2$) for set of 5 specimens	≤ 50 s	≤ 250 s	≤ 250 s
Afterflame + Afterglow time ($t_2 + t_3$) for each specimen	≤ 30 s	≤ 60 s	≤ 60 s
Afterflame or Afterglow of any specimen up to clamp	No	No	No
Cotton indicator ignited by flaming drips	No	No	Yes

The other UL94 test protocols actually result in additional ratings including 5V (the highest flammability performance), HB (the lowest), as well as three other classifications each for horizontally burned specimens and very thin film specimens.

ASTM E2058-09 (Fire Propagation Apparatus)

ASTM's "Standard Test methods for Measurement of Synthetic Polymer Material Flammability Using a Fire Propagation Apparatus" actually uses flames from the burning material itself to characterize fire behavior. Laboratory measurements include heat release taken during upward fire propagation and burning on a vertical test specimen in specific atmospheres (normal air, oxygen rich, and/or oxygen partially depleted). Other measurements include time to ignition, chemical and convective heat release rates for horizontal specimens, mass loss rate and effective heat of combustion. [ASTM E2058-09]. This is the same apparatus referred to for testing the effects of any formulation changes to an FM 4996-approved pallet described above.

ASTM E1354 (ISO 5660) Cone Calorimeter

Unlike some of the above long-lived lab tests, the cone calorimeter is a comparatively newer test used to evaluate and measure rate of heat release of a burning test specimen. In ASTM 1354 (ISO 5660) Standard Test Method for Heat and Visible Smoke Release Rates for Materials and Products Using an Oxygen Consumption Cone Calorimeter, peak and total heat release rates as well as combustion gas composition are assessed in this test and used to characterize the tested materials. See Figure App-VIII-3 for a sketch of the apparatus.

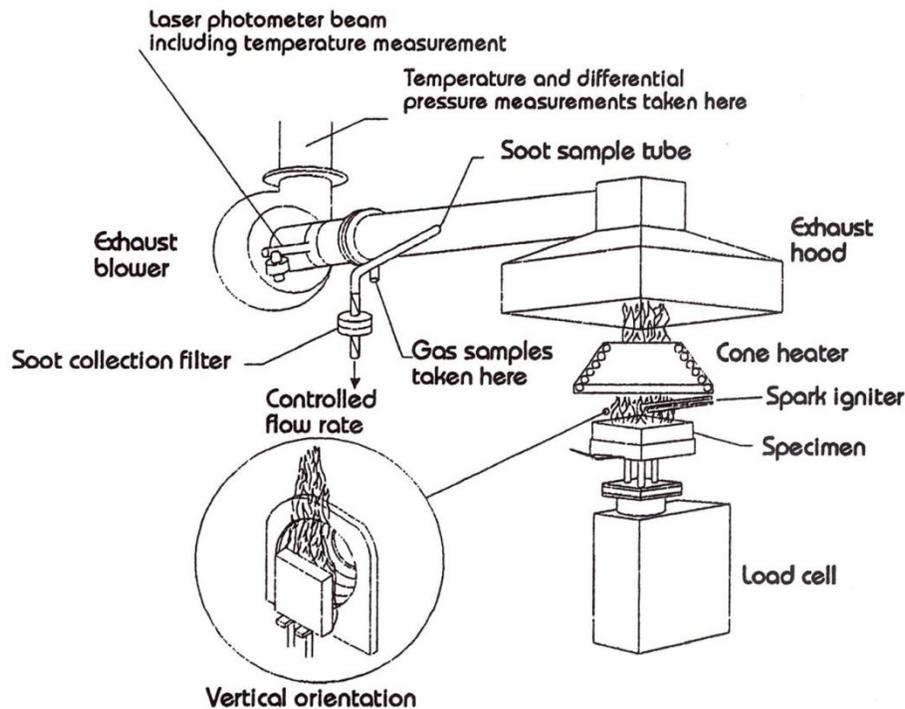


Figure App-VIII-3. Cone Calorimeter Apparatus sketch (Drawing by NIST) (23)

The actual test report includes a total of 24 reported items such as Time to Sustained Flaming (seconds), Heat Release Rate per unit area curve (kW/m^2), Peak and Average Heat Release Rates for 60 seconds, 180 seconds, and 300 seconds after ignition (kW/m^2), Sample Mass Loss (kg/m^2), Smoke Obscuration (average extinction area m^2/kg), and if properly equipped measurements of other combustion gases are also included. [ASTM E1354-04a]

In the authors' opinion, the cone calorimeter and the FM heat release or fire propagation apparatus are the best and possibly the only good test to use in screening a formulation for application in FR plastic pallet. The ultimate requirement in both the FM and UL idle pallet flammability testing is to prove the FR plastic pallet is "like wood" or better. The smaller lab tests like UL94, LOI, etc, are all designed to indicate flame out, not continued burning "like wood". In the cone calorimeter, when wood is evaluated the peak rate of heat release is between $300\text{-}325 \text{ kW}/\text{m}^2$ at 50 kW incident heat. This value provides a benchmark for evaluation of any FR plastic formulation in comparison to wood.

Readers are cautioned that when evaluating in the cone, one flame retardant system can not necessarily be compared to a different flame retardant system. Allowances must be made for differences in fire retardancy mechanism.

The FM Fire Propagation Apparatus could also be used for screening purposes. However, a baseline must be established and the authors have been unable to locate such a baseline in the available literature.

Appendix IX

GREEN SCREEN ALTERNATIVES ASSESSMENTS FOR NINE FLAME RETARDANTS

November 30, 2010



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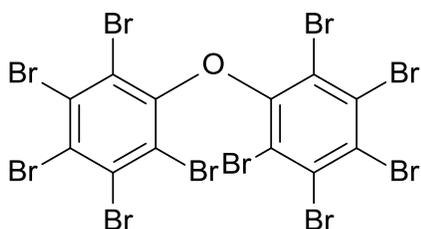
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APPENDIX IXB: GREEN SCREEN FOR DECABROMODIPHENYL ETHER (CAS #1163-19-5)²

Also Called: 1,1'-Oxybis(2,3,4,5,6-pentabromobenzene), 1-06-00-00108 (Beilstein Handbook Reference), AFR 1021, AI3-27894, Adine 505, BDE 209, BDE-209, BR 55N, BRN 2188438, Berkflam B 10E, Bis(pentabromophenyl) ether, Bis(pentabromophenyl)ether, Bromkal 82-0DE, Bromkal 83-10DE, CCRIS 1421, Caliban F/R-P 39P, DB 10, DB 101, DB 102, DE 83, DP 10F, De 83R, Decabrom, Decabromodiphenyl oxide, Decabromobiphenyl ether, Decabromobiphenyl oxide, Decabromodiphenyl ether, Decabromodiphenyl oxide, Decabromophenyl ether, EB 10, EB 10FP, EB 10W, EB 10WS, EBR 700, EINECS 214-604-9, Ether, decabromodiphenyl, F/R-P 53, FR 10, FR 10 (ether), FR 300, FR 300BA, FR-PE, FR-PE(H), FRP 53, Fire Cut 83D, Flame Cut 110R, Flame Cut Br 100, HSDB 2911, NCI-C55287, NSC 82553, Nonnen DP 10, Nonnen DP 10(F), PBED 209, Pentabromophenyl ether, Planelon DB, Planelon DB 100, Planelon DB 101, Plasafety EB 10, Plasafety EBR 700, Saytex 102, Saytex 102E, Tardex 100

Chemical Structure of Decabromodiphenyl Ether:



For Inorganic Chemicals:

Define Form & Physicochemical Properties

1. Particle size (e.g. silica of respirable size) – n/a
2. Structure (e.g. amorphous vs. crystalline) – microcrystalline (NTP 1986)
3. Mobility (e.g. Water solubility, volatility) – 0.1 µg/L at 25°C (Leisewitz 2000)

Identify Applications/Functional Uses: Flame retardant

Green Screen Rating³: Decabromodiphenyl ether was assigned a Benchmark Score of 1 based on a very High persistence (P) rating and High toxicity ratings for both acute (AA) and chronic (CA) aquatic toxicity (1c).

Green Screen (Version 1) Levels of Concern for Decabromodiphenyl Ether														
Human – Tier 1					Human – Tier 2				Eco		Fate		Physical	
C	M	R/D	ED	N	AT	Cr	Sn	ST	AA	CA	P	B	Ex	F
<i>M</i>	<i>L</i>	<i>M</i>	<i>M</i>	<i>M</i>	<i>L</i>	<i>M</i>	<i>L</i>	<i>M</i>	H	H	vH	M	nd	L

*Endpoints in italics were assigned using estimated values and professional judgment (Structure Activity Relationships).

² CPA recommends independent third-party validation of all Green Screen assessments. No independent third-party validation has been done for this assessment. Companies may not make marketing claims based on a Green Screen assessment that has not undergone an independent validation.

³ For inorganic chemicals with low human and ecotoxicity across all hazard endpoints and low bioaccumulation, persistence alone will not be deemed problematic. Inorganic chemicals that are only persistent will be evaluated under the criteria for Benchmark 4.

Transformation Products and Ratings:

Identify relevant fate and transformation products (i.e., dissociation products, transformation products, valence states) and/or moieties of concern⁴

Life Cycle Stage	Transformation Pathway	Transformation Products	CAS #	Green Screen Rating
End of Life	UV Degradation	Low brominated diphenyl oxides	Multiple	n/a
End of Life	UV Degradation	PentaBDE	32534-81-9	PBT (CPA 2009)
End of Life	Combustion	Dioxin	1746-01-6	PBT, Carcinogen, Reproductive/Developmental Toxicant, Neurotoxicant, Endocrine Disruptor (CPA 2009)
End of Life	Combustion	Furan	110-00-9	Carcinogen (CPA 2009)
End of Life	Combustion	Carbon dioxide	124-38-9	Not present on the Red List of Chemicals (CPA 2009)
End of Life	Combustion	Carbon monoxide	630-08-0	Reproductive/Developmental Toxicant, Neurotoxicant (CPA 2009)
End of Life	Combustion	Hydrogen bromide	10035-10-6	Not present on the Red List of Chemicals (CPA 2009)

*The above transformation products were screened against the CPA's table of Red List chemicals.

Introduction

Decabromodiphenyl oxide ("DecaBDE" or "Deca") is an additive flame retardant used in a wide range of polymers including high impact polystyrene, engineering thermoplastics, and textile coating (Leieswitz 2000). DecaBDE has low water solubility (0.1 µg/L at 25°C) and a log K_{ow} of > 5, which indicates a tendency to bioaccumulate. DecaBDE targets the liver, kidneys, spleen, and fat (Leieswitz 2000). The general population may be exposed to decaBDE via inhalation of ambient air, ingestion of fish, and dermal contact with products such as television or computer enclosures or textiles containing decaBDE (HSDB 2010). Studies have shown that all polybrominated diphenyl ethers (PBDEs) bioaccumulate in the environment and that the accumulation is inversely proportional to the degree of bromination (Darnerud 2001). Once in the environment, PBDEs biomagnify in the food chain. Because PBDEs accumulate in fat tissue, high levels of these compounds have been found in fatty fish.

⁴ A moiety is a discrete chemical entity that is a constituent part or component of a substance. A moiety of concern is often the parent substance itself for organic compounds. For inorganic compounds, the moiety of concern is typically a dissociated component of the substance or a transformation product.

DecaBDE is most commonly used as a flame retardant. It is the most common of all polybrominated diphenyl ethers (NAS 2000). The major impurities are isomers of nonabromodiphenyl oxide and octabromodiphenyl oxide. The flame retardant mixture consists of approximately of 66-75% decaBDE and 25-33% antimony trioxide, a synergist (NAS 2000).

Recently, several U.S. states have placed bans on the manufacture or distribution of products containing decaBDE (OECD 2008). The European Union has requested a voluntary reduction program of decaBDE by manufacturers. Under An Act to Clarify Maine's Phaseout of Polybrominated Diphenyl Ethers (Public Laws 2009, chapter 610 [PL 2009, c. 610]), the Maine Department of Environmental Protection (DEP) is currently prohibiting the sale of shipping pallets containing decaBDE unless the pallet is made from recycled shipping pallets or unless an exemption has been granted by the Commissioner of Environmental Protection. The act additionally prohibits the replacement of decaBDE in pallets with other brominated or chlorinated flame retardants. DecaBDE has also been banned from being used in the manufacturing of mattresses and home furniture in Maine and California (OECD 2008).

Human Health – Tier 1

Carcinogenicity (C) Score (H, M or L): M

DecaBDE was assigned a score of Moderate for carcinogenicity based on evidence suggesting the chemical may be carcinogenic in humans and animals.

- DecaBDE has been assigned the following EU risk phrase: R40- Limited evidence of a carcinogenic effect (Physchem 2003).
- Feeding 3,500 to 7,000 mg/kg-bw to mice and 1,200 to 2,400 mg/kg-bw to rats suggests an elevated risk of cancer in the liver, pancreas, thyroid gland as well as an increased risk of leukemia (Leisewitz 2000).
- There is a reported increase in incidence of gullet cancer, rectum carcinoma, and duodenal cancer in decaBDE-exposed workers. However, due to contradictory results, the NTP and IARC have yet to classify decaBDE for carcinogenicity (Leisewitz 2000).
- Groups (50/sex/dose) of F344/N rats and B6C3F1 mice that were fed decaBDE (94–97% pure) at dietary concentrations of 0, 25,000, or 50,000 ppm for 103 weeks (equivalent to 1120, 1200, and 2240 mg/kg-d in male rats; 1120, 1200, and 2550 mg/kg-d in female rats; 3200, 3760, and 6650 mg/kg-d in male mice; and 3200, 3760, and 7780 mg/kg-d in female mice, respectively) Incidences of liver neoplastic nodules were significantly increased in low- and high-dose male rats (7/50 and 15/49, respectively, compared to 1/50 in controls) and high-dose female rats (9/50 compared to 1/50 and 3/49 in control and low-dose groups, respectively); this lesion appeared to be compound related. Incidence of hepatocellular carcinomas was low in all rat groups and apparently not compound related. There was a positive trend in mononuclear cell leukemia in male rats (30/50 controls, 33/50 low-dose rats, 35/50 high-dose rats), but the increase was marginal and not considered to be biologically significant because of the unusually high incidence in controls. A significant positive trend and marginally

greater incidence of acinar cell adenomas in the pancreas of high-dose male rats were also observed, but this lesion was considered to not be compound related. Hepatocellular adenomas or carcinomas (combined) were significantly increased in low- and high-dose male mice (8/50 controls, 22/50 low-dose mice, 18/50 high-dose mice). The incidence of hepatocellular carcinomas alone was significantly elevated in male mice in the low-dose group, but not in the high-dose group, as compared with controls. Thyroid gland follicular cell adenomas or carcinomas (combined) were marginally, but not significantly increased in male mice (0/50 controls, 4/50 low-dose mice, 3/50 high-dose mice). The possible significance of this finding was strengthened by increased incidences of follicular cell hyperplasia in the male mice (2/50 controls, 10/50 low-dose mice, 19/50 high-dose mice), but was weakened by increased mortality in control animals. There was no evidence of carcinogenicity in the female mice at either dose. The study concluded that there was “some evidence of carcinogenicity” for male and female rats based on significantly increased incidences of neoplastic nodules of the liver, and “equivocal evidence of carcinogenicity” for male mice based on a significantly increased incidence of hepatocellular tumors in only the low-dose group and non-statistically significant increases in thyroid follicular cell tumors in both dose groups. The conclusion of “some evidence of carcinogenicity” in rats appears to be based on the finding that the only chemical related effect was benign liver neoplasms. The conclusion of “equivocal evidence of carcinogenicity” in male mice appears to be based on the interpretation that the increases in liver and thyroid tumors are marginal and chemical related (NTP 1986).

Mutagenicity (M) and Genotoxicity Score (H, M or L): L

DecaBDE was assigned a score of Low for mutagenicity based on negative results from several genotoxicity assays.

- DecaBDE tested negative for mutagenicity in *Salmonella typhimurium* tester strains TA 100, TA 1535, TA 1537, and TA 98 at concentrations of 0, 100, 333, 1,000, 3,333, and 10,000 µg/plate with and without metabolic activation (NTP 1986).
- DecaBDE did not induce mutations in mouse L5178Y lymphoma cells with and without S9 at doses of 7, 8, 9, and 10 µg/mL (NTP 1986).
- DecaBDE did not induce sister-chromatid exchanges in Chinese hamster ovary cells both in the presence and absence of S9 at doses of 50, 100, 250, and 500 µg/mL (NTP 1986).
- DecaBDE did not induce chromosomal aberrations in Chinese hamster ovary cells at concentrations of 50, 100, 250, and 500 µg/mL in the presence and absence of S9 (NTP 1986).

Reproductive (R) and Developmental (D) Toxicity Score (H, M or L): M

DecaBDE was assigned a score of Moderate for reproductive and developmental toxicity based on the following risk phrase- R63.

- DecaBDE has been assigned the following EU risk phrase: R63- Possible risk of harm to the unborn child (Lookchem 2008).

- Male (10-15/dose) and female (20-30/dose) Sprague-Dawley rats were administered decaBDE (77.4% pure) daily for 60 days pre-mating, mating, gestation, and lactation for a total of approximately 115 days. Doses were 0, 3, 30, and 100 mg/kg. The reproductive NOAEL was 100 mg/kg (NAS 2000).
- Female rats (strain and number of animals not reported) were administered decaBDE (77.4% pure) at doses of 0, 10, 100, and 1,000 mg/kg on gestation days 6 through 15 via gavage in corn oil. No maternal toxicity or fetal malformations were observed. Subcutaneous edema and delayed skull ossification in pups was observed at 1,000 mg/kg. The maternal NOAEL was 1,000 mg/kg. The fetal NOAEL was 100 mg/kg and the LOAEL was 1,000 mg/kg (NAS 2000).
- Sprague-Dawley rats (25 mated females per dose group) were administered decaBDE in corn oil by gavage at doses of 0, 100, 300, or 1,000 mg/kg-day during gestation days 0 through 19. Dams were sacrificed on day 20 of gestation, and liver weights, gravid uterine weights, and the number of corpora lutea, implants, fetuses, and resorptions were recorded. The placenta and fetuses were examined for gross abnormalities, and histologic examinations were performed. All dams survived decaBDE treatment until scheduled sacrifice. There were no adverse treatment-related effects observed in maternal clinical findings, body weight, or body-weight gain. Although a slight but statistically significant increase in food consumption was observed at 1,000 mg/kg-day at time intervals up to day 12 of gestation, the authors did not consider this indicative of an adverse effect of treatment. No statistically significant differences were observed in maternal absolute or relative liver weights between treatment and control groups. At necropsy, gross examination of the dams revealed no adverse effect of treatment with decaBDE. Number of dams with viable fetuses, mean number of corpora lutea, number of implantation sites, percent preimplantation loss per dam, number of viable fetuses, and gravid uterine weights were not adversely affected by decaBDE treatment. A statistically significant increase in the mean number of early resorptions per dam was observed in the 1,000 mg/kg-day group compared to controls. Based on the lack of a consistent dose response for this effect (the mean number of early resorptions per dam was 0.6, 0.6, 0.5, and 1.4 at 0, 100, 300, and 1,000 mg/kg-day, respectively), lack of a statistically significant positive trend associated with the effect, and the historically high incidence of this effect (0.5–1.4) for the laboratory, these effects are not considered to be of toxicological significance. Examination of the results indicated a marginal increase in the postimplantation loss/dam of 7 and 9% at 300 and 1,000 mg/kg-day, respectively, compared with 4% in controls and at 100 mg/kg-day. However, this effect was not associated with a statistically significant positive trend. A slight, but statistically not significant, decrease in the percentage of viable fetuses per implant was seen (96, 96, 93, and 91% in the control, 100, 300, and 1,000 mg/kg-day groups, respectively). Fetal body weights, crown-rump ratio, and fetal sex ratio were not different between treatment and control groups. No adverse decaBDE treatment-related effects were identified during fetal external, skeletal, or visceral examinations. DecaBDE treatment, therefore, did not produce any evidence of maternal or developmental toxicity up to the highest dose tested of 1,000 mg/kg-day. The NOAEL for maternal and developmental toxicity in this study was 1,000 mg/kg-day, the highest dose tested (IRIS 2008).

Endocrine Disruption (ED) Score (H, M or L): M

DecaBDE was assigned a score of Moderate for endocrine disruption based on the chemical being listed as a potential endocrine disruptor.

- DecaBDE is listed as a potential endocrine disruptor on the EU Priority List of Suspected Endocrine Disruptors.
- DecaBDE is not listed as a potential endocrine disruptor on the OSPAR List of Chemicals of Possible Concern.
- DecaBDE is listed as a potential endocrine disruptor on the Red List of Chemicals (CPA 2009).
- There is suggestive evidence of hypothyroidism in a small number of workers occupationally exposed to decaBDE (ADSTR 2004).
- Long-Evans female rats (eight animals/dose group) were orally administered decaBDE (>98% purity) in corn oil at doses of 0, 0.3, 1, 3, 10, 30, 60, or 100 mg/kg-day for 4 consecutive days. Body weights were recorded and dosing volumes adjusted daily. Animals were sacrificed 1 day after the last dose. Serum total thyroxine (T4) and triiodothyronine (T3), serum thyroid stimulating hormone (TSH), and hepatic enzyme activities (EROD, a marker for CYP-1A1; PROD, a marker for CYP-2B1; and T4-uridine diphosphate glucuronyl transferase [T4-UDPGT]) were measured. Short-term treatment with decaBDE did not cause any visible signs of toxicity or any effects on body-weight gain or liver-to-body-weight ratios at any dose level. DecaBDE (up to 100 mg/kg-day) had no effect on serum T4, T3, or TSH concentration or on hepatic UDPGT activity. Based on these observations, the highest dose of 100 mg/kg-day is identified as the NOAEL (IRIS 2008).

Neurotoxicity (N) Score (H, M or L): M

DecaBDE was assigned a score of Moderate for neurotoxicity based on beings listed as a potential neurotoxicant on the Red List of Chemicals and based on an animal study that suggests decaBDE caused a decrease in activity.

- Not classified as a developmental neurotoxicant (Grandjean and Landrigan 2006).
- DecaBDE is listed as a potential neurotoxicant on the Red List of Chemicals (CPA 2009).
- The neurotoxic effects of decaBDE on spontaneous motor behavior of NMRI male mice were investigated in adult animals exposed to a single oral dose as neonates. Uptake of radiolabel by the brain of the neonatal mice orally administered ¹⁴C-labeled decaBDE on PND 3, 10, or 19 (i.e., at different stages of neonatal mouse brain development) was also measured to determine if there were age-related differences in tissue toxicokinetics that might correlate with the neurodevelopmental effects evaluated. In this behavioral study, 3-day-old and 19-day-old male mice were given a single dose of 0, 2.22, or 20.1 mg/kg body weight decaBDE (purity estimated to be >99%) in a 20% (weight/weight) emulsion vehicle of egg lecithin-peanut oil and water. Ten-day-old mice received 0, 1.34, 13.4, or 20.1 mg/kg. The spontaneous behavior test (measuring locomotion, rearing, and total activity) was conducted in 10 mice randomly selected from the litters in each treatment group at 2, 4, and 6 months of age. Treatment with decaBDE caused no clinical signs of toxicity at any time during the experimental period. Body weight and body-weight gain were not significantly different

between decaBDE- and vehicle-treated mice in the three different age groups. Control mice treated on PND 3, 10, or 19 exhibited normal habituation profiles. Pair-wise testing between adult mice exposed to 20.1 mg/kg on PND 3 and control groups indicated significant changes in all three spontaneous behavior variables at 2, 4, and 6 months of age. For the first 20 minutes, mice receiving 20.1 mg/kg displayed significantly less activity for locomotion, rearing, and total activity compared with controls. During the third 20-minute period, exposure of mice to 20.1 mg/kg on PND 3 caused significantly more activity for locomotion, rearing, and total activity than the controls at 2, 4, and 6 months. The only effect noted in mice exposed to 2.22 mg/kg was a significant decrease in total activity in the first 20-minute test period compared with the controls at 2 months of age. However, total activity returned to control level during the third 20-minute period. The lower dose of 2.22 mg/kg did not elicit any significant differences in these three variables compared with controls at 4 months of age. Lower activity was observed at 2.22 mg/kg during the first 20-minute period for the rearing variable at 6 months of age compared with controls, again returning to control level during the third 20-minute period. Mice exposed neonatally up to 20.1 mg on either PND 10 or 19 did not show any significant differences in any of the variables after 2, 4, or 6 months compared with controls. The authors indicated that the absence of effects on spontaneous activity in mice treated on PNDs 10 and 19 suggests that there is a critical window for the induction of the observed behavioral disturbances. The NOAEL in this study was 2.22 mg/kg, and the LOAEL was 20.1 mg/kg for significant changes in spontaneous motor behavior and decreased habituation capability for locomotion, rearing, and total activity, worsening with increasing age (IRIS 2008).

Human Health – Tier 2

Acute Mammalian (AT) Toxicity Score (H, M or L): L

DecaBDE was assigned a score of Low for acute mammalian toxicity based on oral and dermal LD₅₀ values greater than 2,000 mg/kg-bw. Data is from three different routes of exposure in two different species of animals.

- DecaBDE has low acute oral toxicity because it is poorly absorbed from the gastrointestinal tract (NAS 2000).
- *Oral*: An LD₅₀ of > 2,000 mg/kg was determined in the rat (ESIS 2000).
- *Oral*: An LD₅₀ of > 5,000 mg/kg was determined in the rat (ESIS 2000).
- *Dermal*: An LD₅₀ of > 2,000 mg/kg was determined in the rabbit (ESIS 2000).
- *Inhalation*: An LC₅₀ of > 48.2 mg/L was determined in the rat (ESIS 2000).
- *Inhalation*: No deaths occurred in groups of 5 male and 5 female rats chamber-exposed to decaBDE dust mixture at concentrations as high as 48,200 mg/m³ for 1 hour and observed the following 14 days (ATSDR 2004).

Corrosion/ Irritation (Skin/ Eye) (Cr) Score (H, M or L): M

DecaBDE was assigned a score of Moderate for corrosion and irritation based on the following risk phrases: R36, R37, R38.

- DecaBDE has been assigned the following EU risk phrases: R36- Irritating to eyes, R37- Irritating to respiratory tract, R38- Irritating to skin (Physchem 2003).
- Although animal studies have shown decaBDE to not be corrosive or irritating, occupational reports have suggested the substance produces skin and eye irritation (Leisewitz 2000).
- *Dermal*: DecaBDE caused essentially no dermal response in rabbits when applied as a dry solid (500 mg) to intact shaved skin under occluded conditions for 24 hours, and a slight erythematous and edematous response when similarly applied to abraded skin. Repeated application of dry solid decaBDE (500 mg) to intact skin of rabbits for 5 days/week for 2 weeks or to abraded skin for 3 days also did not alter their dermal responses (NAS 2000).
- *Dermal*: An acnegenesis study was performed in which 0.1 mL of 0.1%, 1%, 10%, or 100% decaBDE (0.40 mg/kg) in chloroform was rubbed into the external ear canal of four rabbits/dose level once a day, 5 days/week for 4 weeks. Observations made prior to the initial dose and after 7, 14, 21, and 28 days of dosing showed slight erythema, epidermal sloughing and scaling (effect levels not specified), but no clear indication of chloracne (a slight response was observed in one animal at the 10% concentration on day 28). Gross necropsy showed no treatment-related systemic effects. Other studies similarly reported that a 10% chloroform solution of decaBDE caused slight erythema and exfoliation, and no indication of chloracne, when applied to the ear of rabbits for 28 days. Other industry studies also found that 10% decaBDE in chloroform did not induce chloracne in rabbits (NAS 2000).
- *Ocular*: Ocular exposure to dry solid decaBDE caused transient conjunctival irritation in washed and unwashed rabbit eyes. Instillation of decaBDE (100 mg/eye) into the eye caused very slight conjunctival redness and chemosis and slight or moderate discharge in some rabbits, but the investigators concluded that the effects were not serious enough to be considered primary eye irritation. Other studies similarly reported that decaBDE did not cause primary eye irritation when instilled once (100 mg/eye) into the eye of rabbits (NAS 2000).
- *Ocular*: Rats (strain and number not reported) that were chamber-exposed to decaBDE dust at concentrations of 48,200 mg/m³ for one hour showed signs of eye squint, erythema, and/or ocular discharge (ADSTR 2004).

Sensitization (Sn) Score (Skin and Respiratory) (H, M or L): L

DecaBDE was assigned a score of Low for sensitization based on negative results from human and animal studies.

- *Dermal*: DecaBDE does not appear to be a primary irritant based on observations from a skin sensitization study in humans and dermal irritation and acnegenesis studies in animals. A human skin sensitization study was conducted in which 0.03 mL of a 5% suspension of commercial decaBDE in petrolatum (0.02 mg/kg) was applied via patch to the skin of 50 subjects three times per week for 3 weeks. Commercial decaBDE was a mixture that contained 77.4% decaBDE, 21.8% nonaBDE, and 0.8% octoBDE. The dermal applications did not result in skin sensitization reactions during the sensitizing period or on challenge 2 weeks after the last application. Skin irritation, attributed to the stringency of the test procedure by the investigators, occurred in 9 of the 50 subjects (14/450 total

applications; 11 of the reactions were classified as very slight and 3 as mild erythema) (NAS 2000).

Systemic/ Organ (ST) Toxicity Score (includes organ effects and immunotoxicity) (H, M or L): M

DecaBDE was assigned a score of Moderate for systemic toxicity based on animal studies and the following risk phrases: R20, R21, R22, R48/20.

- DecaBDE has been assigned the following EU risk phrases: R20- Harmful by inhalation, R21- Harmful in contact with skin, R22- Harmful if swallowed (Physchem 2003) and R48/20- Danger of serious damage to health by prolonged exposure and harmful by inhalation (Lookchem 2008).
- DecaBDE will accumulate in the liver, kidneys, and fat tissue of animals (Leisewitz 2000).
- Rats (strain, sex, and number of animals not reported) were exposed to decaBDE at concentrations of 2,000 or 48,000 mg/m³ via inhalation for 1 hour and then observed for 14 days. No deaths or effects on body weight were observed however, dyspnea and ocular porphyrin discharge were observed at both concentration levels and eye squint was observed in the high concentration level only (NAS 2000).
- Male Sprague-Dawley rats (5/dose) were administered oral doses of decaBDE (77.4% pure) at 0, 8, 80, and 800 mg/kg per day for 30 days. Clinical symptoms included thyroid hyperplasia at the 80 and 800 mg/kg dose levels, increased liver weight at 80 mg/kg, increased liver weight and pathology at 800 mg/kg, and renal tubular degeneration at 800 mg/kg. A NOAEL of 8 mg/kg-day and LOAEL of 80 mg/kg-day was assigned (NAS 2000).
- Male and female rats (10/dose, strain not reported) were administered decaBDE (purity not reported) orally in doses of 0, 7.4, or 74 mg/kg-day for 28 days. No histological liver or thyroid changes were observed and the NOAEL was established to be 74 mg/kg-day (NAS 2000).
- In a 2 year oral study, male and female Sprague-Dawley rats (25/dose) were administered decaBDE (77.4% pure) at concentrations of 0, 0.01, 0.1, or 1 mg/kg-day. No adverse effects were observed and the NOAEL was established to be 1 mg/kg-day (NAS 2000).
- Male and female F344/N rats (5/sex/dose) were fed diets containing 0, 5,000, 10,000, 20,000, 50,000, or 100,000 ppm decaBDE (99% purity) for 14 days. The corresponding estimated average daily doses were 0, 472, 928, 1,846, 4,569, or 9,326 mg/kg-day in male rats and 0, 538, 1,061, 2,137, 5,323, or 10,853 mg/kg-day in female rats. No mortality was observed in the rats during the course of the study. Exposure to decaBDE did not cause any clinical signs of toxicity or adversely affect the final mean body weights. Gross pathological effects were not noted in any animal at any dose level. The results of this study indicated a NOAEL of 9,326 mg/kg-day in male rats and 10,853 mg/kg-day in female rats (NTP 1986).
- The subchronic effects of decaBDE (97–99% purity) on rats were investigated in a 13-week study. Groups of F344/N rats (10/sex/dose) were administered decaBDE in the diet at concentrations of 0, 3,100, 6,200, 12,500, 25,000, or 50,000 ppm for 13 weeks. The corresponding estimated average daily doses were

- 0, 191, 372, 781, 1,536, or 3,066 mg/kg-day in male rats and 0, 238, 504, 967, 1,955, or 3,944 mg/kg-day in female rats. A necropsy was performed on all animals, including those killed in extremis, with the exception of those excessively autolyzed or cannibalized. Histologic examination was performed on major organs and tissues from control and high-dose groups. No mortality was observed in rats fed decaBDE, and no clinical signs of toxicity were noted. Compound-related changes in body weight and feed consumption were not observed, and no gross or macroscopic pathological effects were noted in any animal examined. The results indicate a NOAEL of 3,066 mg/kg-day in male rats and 3,944 mg/kg-day in female rats (NTP 1986).
- Male and female B6C3F1 mice (5/sex/dose) were fed diets containing 0, 5,000, 10,000, 20,000, 50,000, or 100,000 ppm decaBDE (99% purity) for 14 days. The estimated average daily doses were 0, 1,027, 2,143, 4,246, 10,536, or 20,994 mg/kg-day in male mice and 0, 1,146, 2,286, 4,627, 11,348, or 23,077 mg/kg-day in female mice. Necropsy was performed at the end of the exposure period, and several organs and tissues were examined histologically. Exposure to decaBDE up to 20,994 mg/kg-day in males and 23,077 mg/kg-day in females showed no effects on survival or body weight, and there were no clinical signs of toxicity. No compound-related gross pathological effects were noted in any animal in any group. The results of this study indicate a NOAEL of 20,994 mg/kg-day in male mice and 23,077 mg/kg-day in female mice (NTP 1986).
 - B6C3F1 mice (10/sex/dose) were fed diets containing 0, 3,100, 6,300, 12,500, 25,000, or 50,000 ppm decaBDE (97–99% purity) for 13 weeks. The corresponding estimated average daily doses were 0, 666, 1,355, 2,659, 5,278, or 10,233 mg/kg-day in males and 0, 702, 1,437, 2,899, 5,687, or 11,566 mg/kg-day in females. Necropsy was performed on all animals, including those killed in extremis, with the exception of those excessively autolyzed or cannibalized. Histologic examination was performed on the organs and tissues from control and high-dose groups. Only one male and one female mouse fed 12,500 ppm died in the course of the study. There were no clinical signs of toxicity, and no compound-related effects on body weight and feed consumption were observed. No gross or macroscopic pathological effects were noted in any animal at any dose. The results of this study indicated a NOAEL of 10,233 mg/kg-day in males and 11,566 mg/kg-day in females (NTP 1986).

Ecotoxicity

Acute Aquatic (AA) Toxicity Score (H, M or L): H

DecaBDE was assigned a score of High for acute aquatic toxicity based on L/EC₅₀ values less than 1 mg/L.

- An LC₅₀ of > 500 mg/L was identified in killifish (freshwater fish, 48 hour) (ESIS 2000).
- ECOSAR – DecaBDE is designated to the neutral organics ECOSAR class. The estimated L/EC₅₀ values are 9.4x10⁻⁷ mg/L (fish, 96 hr), 2.36x10⁻⁶ mg/L (daphnid, 48 hr), and 9.05x10⁻⁵ mg/L (algae, 96 hr) (U.S. EPA 2009).
- An EC₅₀ of > 1 mg/L was identified in algae (ESIS 2000).

Chronic Aquatic (CA) Toxicity Score (H, M or L): H

DecaBDE was assigned a score of High for chronic aquatic toxicity based on ChV values less than 0.1 mg/L.

- DecaBDE has been assigned the following EU risk phrase: R50/53- Very toxic to aquatic organisms, may cause long term effects in the aquatic environment (Lookchem 2008).
- ECOSAR – The estimated ChV values are 6.06×10^{-7} mg/L (fish, 96 hr) and 1.36×10^{-6} mg/L (daphnid) (U.S. EPA 2009).

Environmental Fate**Persistence (P) Score (vH, H, M, or L): vH**

DecaBDE was assigned a score of very High for persistence based on the chemical not being readily biodegradable and a half life in soil greater than 180 days and a half life in water greater than 60 days.

- BIOWIN predicts decabDE will not readily biodegrade. STP removal expected using BIOWIN/EPA Draft Method results indicate 94.04% total removal, with 0.78% due to biodegradation. Fugacity modeling predicts 95.6% partitioning to soil with a half-life of 360 days, and 4.26% partitioning to water with a half-life of 180 days (U.S. EPA 2010).

Bioaccumulation (B) Score (vH, H, M, or L): M

DecaBDE was assigned a score of Moderate for bioaccumulation based on a BAF less than 500, and a log K_{ow} greater than 5, and degradation products that are likely to bioaccumulate.

- BCFBAF predicts a bioaccumulation factor (BAF) of 6.929 and a log K_{ow} of 12.11 (U.S. EPA 2010).

Physical Properties**Explosivity (Ex) Hazard Rating (H, M or L): nd**

- No relevant data were identified for DecaBDE.

Flammability (F) Hazard Rating (H, M or L): L

DecaBDE was assigned a score of Low for flammability because no basis for concern was identified.

- DecaBDE is not flammable (ESIS 2000).

EPI Suite Results for Decabromodiphenyl Ether:

CAS Number: 1163-19-5

SMILES : O(c(c(c(c(c1Br)Br)Br)Br)c1Br)c(c(c(c(c2Br)Br)Br)Br)c2Br

CHEM : Benzene, 1,1 -oxybis[2,3,4,5,6-pentabromo-

MOL FOR: C12 Br10 O1

MOL WT : 959.17

----- EPI SUMMARY (v4.00) -----

Physical Property Inputs:

Log Kow (octanol-water): -----

Boiling Point (deg C) : -----

Melting Point (deg C) : -----

Vapor Pressure (mm Hg) : -----

Water Solubility (mg/L): -----

Henry LC (atm-m³/mole) : -----

Log Octanol-Water Partition Coef (SRC):

Log Kow (KOWWIN v1.67 estimate) = 12.11

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPVP v1.43):

Boiling Pt (deg C): 589.71 (Adapted Stein & Brown method)

Melting Pt (deg C): 254.50 (Mean or Weighted MP)

VP(mm Hg,25 deg C): 4.67E-012 (Modified Grain method)

VP (Pa, 25 deg C) : 6.23E-010 (Modified Grain method)

MP (exp database): 295 deg C

BP (exp database): 530 deg C

Subcooled liquid VP: 4.74E-009 mm Hg (25 deg C, Mod-Grain method)

: 6.32E-007 Pa (25 deg C, Mod-Grain method)

Water Solubility Estimate from Log Kow (WSKOW v1.41):

Water Solubility at 25 deg C (mg/L): 2.841e-011

log Kow used: 12.11 (estimated)

no-melting pt equation used

Water Sol (Exper. database match) = 0.0001 mg/L (25 deg C)

Exper. Ref: HARDY,ML & SMITH,RL (1999); < 0.1 ppb

Water Sol Estimate from Fragments:

Wat Sol (v1.01 est) = 2.5606e-006 mg/L

ECOSAR Class Program (ECOSAR v1.00):

Class(es) found: Neutral Organics

Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:

Bond Method : 1.19E-008 atm-m³/mole (1.20E-003 Pa-m³/mole)

Group Method: 4.45E-008 atm-m³/mole (4.51E-003 Pa-m³/mole)

For Henry LC Comparison Purposes:

User-Entered Henry LC: not entered

Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:

HLC: 2.075E-001 atm-m³/mole (2.102E+004 Pa-m³/mole)

VP: 4.67E-012 mm Hg (source: MPBPVP)

WS: 2.84E-011 mg/L (source: WSKOWWIN)

Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1.10]:

Log Kow used: 12.11 (KowWin est)

Log Kaw used: -6.313 (HenryWin est)

Log Koa (KOAWIN v1.10 estimate): 18.423

Log Koa (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10):

Biowin1 (Linear Model) : -0.6806

Biowin2 (Non-Linear Model) : 0.0000

Expert Survey Biodegradation Results:

Biowin3 (Ultimate Survey Model): -0.3386 (recalcitrant)

Biowin4 (Primary Survey Model) : 1.0059 (recalcitrant)

MITI Biodegradation Probability:

Biowin5 (MITI Linear Model) : -0.2784

Biowin6 (MITI Non-Linear Model): 0.0001

Anaerobic Biodegradation Probability:

Biowin7 (Anaerobic Linear Model): 1.0141

Ready Biodegradability Prediction: NO

Hydrocarbon Biodegradation (BioHCwin v1.01):

Structure incompatible with current estimation method!

Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:

Vapor pressure (liquid/subcooled): 6.32E-007 Pa (4.74E-009 mm Hg)

Log Koa (Koawin est): 18.423

Kp (particle/gas partition coef. (m³/ug)):

Mackay model : 4.75

Octanol/air (Koa) model: 6.5E+005

Fraction sorbed to airborne particulates (phi):

Junge-Pankow model : 0.994

Mackay model : 0.997

Octanol/air (Koa) model: 1

Atmospheric Oxidation (25 deg C) [AopWin v1.92]:

Hydroxyl Radicals Reaction:

OVERALL OH Rate Constant = 0.0337 E-12 cm³/molecule-sec

Half-Life = 317.534 Days (12-hr day; 1.5E6 OH/cm³)

Ozone Reaction:

No Ozone Reaction Estimation

Fraction sorbed to airborne particulates (phi):

0.996 (Junge-Pankow, Mackay avg)

1 (Koa method)

Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (KOCWIN v2.00):

Koc : 2.762E+005 L/kg (MCI method)

Log Koc: 5.441 (MCI method)

Koc : 4.78E+007 L/kg (Kow method)

Log Koc: 7.679 (Kow method)

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v2.00]:

Rate constants can NOT be estimated for this structure!

Bioaccumulation Estimates (BCFBAF v3.00):

Log BCF from regression-based method = 1.620 (BCF = 41.71 L/kg wet-wt)

Log Biotransformation Half-life (HL) = 2.7638 days (HL = 580.5 days)

Log BCF Arnot-Gobas method (upper trophic) = -0.039 (BCF = 0.9147)

Log BAF Arnot-Gobas method (upper trophic) = 0.841 (BAF = 6.929)

log Kow used: 12.11 (estimated)

Volatilization from Water:

Henry LC: 4.45E-008 atm-m³/mole (estimated by Group SAR Method)
 Half-Life from Model River: 4.075E+004 hours (1698 days)
 Half-Life from Model Lake : 4.448E+005 hours (1.853E+004 days)

Removal In Wastewater Treatment:
 Total removal: 94.04 percent
 Total biodegradation: 0.78 percent
 Total sludge adsorption: 93.26 percent
 Total to Air: 0.00 percent
 (using 10000 hr Bio P,A,S)

Removal In Wastewater Treatment:
 Total removal: 94.04 percent
 Total biodegradation: 0.78 percent
 Total sludge adsorption: 93.26 percent
 Total to Air: 0.00 percent
 (using Biowin/EPA draft method)

Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.114	7.62e+003	1000
Water	4.26	4.32e+003	1000
Soil	95.6	8.64e+003	1000
Sediment	0.00236	3.89e+004	0

 Persistence Time: 7.26e+003 hr

ECOSAR Results for Decabromodiphenyl Ether:

SMILES : O(c(c(c(c(c1Br)Br)Br)Br)c1Br)c(c(c(c(c2Br)Br)Br)Br)c2Br
 CHEM : Benzene, 1,1 -oxybis[2,3,4,5,6-pentabromo-
 CAS Num: 001163-19-5
 ChemID1:
 ChemID2:
 ChemID3:
 MOL FOR: C12 Br10 O1
 MOL WT : 959.17
 Log Kow: 12.11 (KowWin estimate)
 Melt Pt:
 Wat Sol: 0.0001 mg/L (experimental database)

ECOSAR v1.00 Class(es) Found

 Neutral Organics

ECOSAR Class	Organism	Predicted		
		Duration	End Pt	mg/L (ppm)
Neutral Organics	: Fish	96-hr	LC50	9.4e-007
Neutral Organics	: Fish	14-day	LC50	1.12e-006
Neutral Organics	: Daphnid	48-hr	LC50	2.36e-006
Neutral Organics	: Green Algae	96-hr	EC50	9.05e-005
Neutral Organics	: Fish	30-day	ChV	1.93e-007
Neutral Organics	: Daphnid		ChV	1.36e-006
Neutral Organics	: Green Algae		ChV	0.000187 *
Neutral Organics	: Fish (SW)	96-hr	LC50	6.06e-007
Neutral Organics	: Mysid Shrimp	96-hr	LC50	6.92e-010

Neutral Organics	: Fish (SW)	ChV	4.57e-005
Neutral Organics	: Mysid Shrimp (SW)	ChV	2.99e-012
Neutral Organics	: Earthworm	14-day LC50	149.184 *

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect.

Neutral Organics:

For Fish LC50 (96-h), Daphnid LC50, Mysid: If the log Kow is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

For Fish LC50 (14-day) and Earthworm LC50: If the log Kow is greater than 6.0, or if the compound is solid and the LC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

For Green Algae Acute Toxicity Values: If the log Kow of the chemical is greater than 6.4, or if the compound is solid and the EC50 exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

For All Chronic Toxicity Values: If the log Kow of the chemical is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

ECOSAR v1.00 SAR Limitations:

Maximum LogKow: 5.0 (Fish 96-hr LC50; Daphnid LC50, Mysid LC50)
Maximum LogKow: 6.0 (Fish 14-day LC50; Earthworm LC50)
Maximum LogKow: 6.4 (Green Algae EC50)
Maximum LogKow: 8.0 (ChV)
Maximum Mol Wt: 1000

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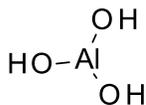


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APPENDIX IX C: GREEN SCREEN FOR ALUMINUM TRIHYDROXIDE (CAS #21645-51-2)⁵

Also Called: Aluminum oxide trihydrate, Aluminum trihydroxide, Alumina trihydrate, Aluminic acid

Chemical Structure of Aluminum Trihydroxide:



For Inorganic Chemicals:

Define Form & Physiochemical Properties (Leisewitz 2001)

1. Particle size: 0.1-0.6 μm
2. Structure: Crystalline
3. Mobility: Insoluble in water; soluble in alkaline solutions, acid solutions

Identify Applications/Functional Uses: Flame retardant

Green Screen Rating⁶: Aluminum trihydroxide was assigned a Green Screen Benchmark Score of 2 based on very High persistence (P), Moderate neurotoxicity (N), Moderate systemic toxicity (ST), and Moderate corrosion/irritation (Cr) (2c).

Green Screen (Version 1) Levels of Concern for Aluminum Trihydroxide														
Human – Tier 1					Human – Tier 2				Eco		Fate		Physical	
C	M	R/D	ED	N	AT	Cr	Sn	ST	AA	CA	P	B	Ex	F
L	<i>L</i>	L	nd	M	L	M	L	M	L	<i>M</i>	vH	L	L	L

*Endpoints in italics were assigned using estimated values and professional judgment (Structure Activity Relationships).

⁵ CPA recommends independent third-party validation of all Green Screen assessments. No independent third-party validation has been done for this assessment. Companies may not make marketing claims based on a Green Screen assessment that has not undergone an independent validation.

⁶ For inorganic chemicals with low human and ecotoxicity across all hazard endpoints and low bioaccumulation, persistence alone will not be deemed problematic. Inorganic chemicals that are only persistent will be evaluated under the criteria for Benchmark 4.

Transformation Products and Ratings:

Identify relevant fate and transformation products (i.e., dissociation products, transformation products, valence states) and/or moieties of concern⁷

Life Cycle Stage	Transformation Pathway	Transformation Products	CAS #	Green Screen Rating
End of life	Dissociation	Al ³⁺	7429-90-5	Present on the Red List of chemicals (CPA 2009).
End of life	Dissociation	OH-	3352-57-6	Not present on the Red List of chemicals (CPA 2009).

*The above transformation products were screened against the CPA's table of Red List chemicals.

Introduction

Aluminum trihydroxide is an additive mineral flame retardant, filler, and an additive for fume reduction (Leisewitz 2001). Because it is a relatively weak-acting flame retardant, it must be utilized in large quantities, which limits its application area. In addition, aluminum trihydroxide decomposes at 200°C which further limits its application and cannot be used in plastics with high processing temperatures.

Aluminum trihydroxide is primarily used in the manufacturing of glass, ceramics, activated alumina, flame retardants and mattress bedding. It is also used as a rubber reinforcing agent, paper coating, filler, and in cosmetics. Aluminum trihydroxide is also used as an antacid and an antihyperphosphatemic (Lewis 1997).

Human Health – Tier 1

Carcinogenicity (C) Score (H, M or L): L

Aluminum trihydroxide was assigned a score of Low for carcinogenicity based on results from animal studies.

- Not classifiable as a human carcinogen (ACGIH 2008).
- Aluminum hydroxide was not carcinogenic after daily intraperitoneal administration to mice for 4 months at dosages up to 200 mg/kg/day (FAO/WHO 1989).

⁷ A moiety is a discrete chemical entity that is a constituent part or component of a substance. A moiety of concern is often the parent substance itself for organic compounds. For inorganic compounds, the moiety of concern is typically a dissociated component of the substance or a transformation product.

- In a 6 month study in rats the effects of aluminum on renal function were and phosphate handling were studied. Rats (number/strain not reported) were given aluminum hydroxide (80 mg/kg, IP) 3 times/wk. No changes were observed in renal function and no evidence of carcinogenicity was found (Mahieu 1998).

Mutagenicity (M) and Genotoxicity Score (H, M or L): L

No mutagenicity and genotoxicity data were identified for aluminum hydroxide. A score of Low was assigned based on the U.S. EPA's assessment on flame retardants in printed circuit boards for aluminum hydroxide (U.S. EPA 2008).

- No relevant data on mutagenicity was identified for aluminum hydroxide.
- Aluminum hydroxide is estimated to be of low genotoxic potential (U.S. EPA 2008).

Reproductive (R) and Developmental (D) Toxicity Score (H, M or L): L

Aluminum trihydroxide was assigned a score of Low for reproductive and developmental toxicity based on negative results from animal studies.

- When high doses (≤ 1094 mg/kg/day) of aluminum hydroxide were orally administered to pregnant rats and mice during embryogenesis, no maternal or developmental toxicity occurred (Bingham 2001).
- No developmental effects occurred in Swiss mice (number not reported) at doses of 66.5, 133, or 266 mg/kg/day following gavage administration on gestation days 6-15 (Domingo 1989).
- No developmental toxicity occurred in Swiss albino CD-1 mice (number not reported) at a dose of 57.5 mg/kg/day following gavage administration on gestation days 6-15 (Colomina 1992).
- No developmental toxicity occurred in Sprague-Dawley rats (number not reported) at a gavage dose of 384 mg/kg/day on gestation days 6-15 (Gomez 1991).
- No developmental toxicity occurred in Wistar rats (number not reported) at gavage doses of 192, 384, and 768 mg/kg/day (Gomez 1990).

Endocrine Disruption (ED) Score (H, M or L): nd

- Aluminum trihydroxide is not listed as a potential endocrine disruptor on the EU Priority List of Suspected Endocrine Disruptors.
- Aluminum trihydroxide is not listed as a potential endocrine disruptor on the OSPAR List of Chemicals of Possible Concern.
- Aluminum trihydroxide is not listed as a potential endocrine disruptor on the Red List of Chemicals (CPA 2009).

Neurotoxicity (N) Score (H, M or L): M

Aluminum trihydroxide was assigned a score of Moderate for neurotoxicity based on results from animal studies and being present on the red list as a potential neurotoxicant.

- In a 30-day study rats (number/strain not reported) were fed aluminum in an oral diet with no significant effects noted and a reported NOAEL of 1252 mg/kg/day (ASTDR 2008).

- In a 90-day study rats (number/strain not reported) were given aluminum hydroxide with citric acid by oral gavage and demonstrated impaired learning in a labyrinth maze test. A LOAEL of 35 mg/kg/day was reported (ASTDR 2008).
- Aluminum hydroxide is expected to be of moderate hazard for neurotoxicity based on available data (U.S. EPA 2008).

Human Health – Tier 2

Acute Mammalian (AT) Toxicity Score (H, M or L): L

A score of Low for acute mammalian toxicity was assigned to aluminum trihydroxide based on an oral LD₅₀ value greater than 5,000 mg/kg-bw. Data is from one route of exposure in two different species.

- *Oral*: TDLo (child) = 79,000 mg/kg (ChemIDplus 2010)
- *Oral*: TDLo (child) = 122,000 mg/kg (ChemIDplus 2010)
- *Oral*: LD₅₀ (rat) > 5,000 mg/kg (ESIS 2000)

Corrosion/ Irritation (Skin/ Eye) (Cr) Score (H, M or L): M

Aluminum trihydroxide was assigned a score of Moderate for corrosion and irritation based on human studies and MSDS data.

- Aluminum trihydroxide may cause mild skin, eye and upper respiratory tract irritation (ScienceLab 2010).

Sensitization (Sn) Score (Skin and Respiratory) (H, M or L): L

Aluminum trihydroxide was assigned a score of Low for sensitization based on aluminum hydroxide testing negative for skin and respiratory sensitization.

- *Dermal*: Aluminum trihydroxide was not sensitizing. No other details were provided (ESIS 2000).
- *Respiratory/Dermal*: Aluminum trihydroxide was not sensitizing. No other details were provided (ESIS 2000).

Systemic/ Organ (ST) Toxicity Score (includes organ effects and immunotoxicity) (H, M or L): M

Aluminum trihydroxide was assigned a score of Moderate for systemic/organ toxicity based on potential immunotoxic effects in humans.

- The effects of dietary administration of aluminum hydroxide were examined in male Sprague-Dawley rats. Groups of 25 rats were fed a diet containing 14,470 ppm aluminum hydroxide or a control diet for 28 days. The mean daily aluminum dose was calculated as 302 mg/kg body weight/day. Dietary administration of aluminum hydroxide did not induce any signs of toxicity. Clinical observations during the 28-day treatment period and the recovery phase were similar in control and treated rats. There were no significant changes in hematology, clinical chemistry parameters, or organ weights (Hicks 1987).

- In a 6-week oral administration study in humans, a reduction in primed cytotoxic T-cells was observed and a LOAEL of 25 mg/kg/day was reported (ATSDR 2008).

Ecotoxicity

Acute Aquatic (AA) Toxicity Score (H, M or L): L

Aluminum trihydroxide was assigned a score of Low for acute aquatic toxicity based on LC₅₀ values greater than 100 mg/L.

- 96-hour LC₅₀ (*fish*) > 100 mg/L (ESIS 2000)
- 48-hour LC₅₀ (*Daphnia magna*) > 100 mg/L (ESIS 2000)
- 72-hour EC₅₀ (*Selenastrum capricornutum*) > 100 mg/L (ESIS 2000)

Chronic Aquatic (CA) Toxicity Score (H, M or L): M

No data was identified for aluminum trihydroxide. Aluminum trihydroxide was assigned a score of Moderate chronic aquatic toxicity based GHS criteria for chronic aquatic toxicity.

- There were no data identified on the chronic aquatic toxicity of aluminum hydroxide. The globally harmonized system (GHS) Categorization of poorly soluble substances for which no chronic or acute toxicity data exist are classified as chronic aquatic toxicity category 4, a “safety net” category. The Green Screen assigns these chemicals a rating of “moderate.”

Environmental Fate

Persistence (P) Score (vH, H, M, or L): vH

Aluminum trihydroxide was assigned a score of very High for persistence based on the chemical being an inorganic compound and not having any identifiable biodegradation pathways at normal environmental conditions.

- As an oxidized inorganic compound, aluminum trihydroxide is not expected to biodegrade, oxidize further in air, or undergo hydrolysis at environmental conditions. No degradation process for aluminum trihydroxide could be identified at typical environmental conditions (US EPA 2008).

Bioaccumulation (B) Score (vH, H, M, or L): L

Aluminum trihydroxide was assigned a score of Low for bioaccumulation based on a BCF value less than 100.

- Aluminum hydroxide has a predicted BCF of 3.2 (U.S. EPA 2008).
- Aluminum hydroxide is not expected to be bioaccumulative (U.S. EPA 2008).

Physical Properties

Explosivity (Ex) Hazard Rating (H, M or L): L

Aluminum trihydroxide was assigned a Low for explosivity because no basis for concern was identified.

- Aluminum hydroxide is not explosive (ESIS 2000)

Flammability (F) Hazard Rating (H, M or L): L

Aluminum trihydroxide was assigned a Low for flammability because no basis for concern was identified.

- Aluminum hydroxide is not flammable (ESIS 2000)

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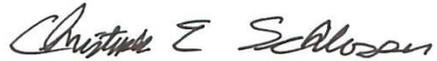
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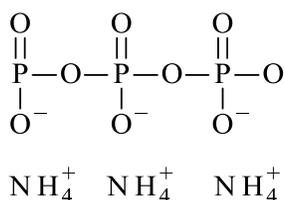


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APPENDIX IX D: GREEN SCREEN FOR AMMONIUM POLYPHOSPHATE (CAS #68333-79-9)⁸

Also Called: AP 422, AP 462, APP (fireproofing agent), APP 422, Albaplas AP 95, Aluminum polyphosphate, Amgard CL, Amgard MC, Amgard TR, Ammonium ortho and polyphosphate solution, Ammonium orthophosphate, superphosphate, Ammonium polyphosphate, Ammonium polyphosphates, Antiblaze MC, Antiblaze MCM, Budit 3076, Budit 3076DC, Budit 3077, Budit 365, DFP-I, EINECS 269-789-9, EXO 462, Exolit 263, Exolit 422, Exolit 442, Exolit 454, Exolit 455, Exolit 462, Exolit 470, Exolit AP 422, Exolit AP 423, Exolit AP 462, FR-Cros 480, FR-Cros 484, Fire-Trol LCG-R, Flameguard PT 8, Hostaflam 423, Hostaflam AP 420, Hostaflam AP 422, Hostaflam AP 462, Hostaflam AP 464, Hostaflam TP-AP 751, Hostaflam TP-AP 752, Novawhite, Phos-Chek P 30, Phos-Chek P 40, Phos-Chek P 60, Poly-N 10-34-0, Poly-N 11-37-0, Polymetaphosphoric acid, ammonium salt, Polyphosphoric acid, ammonium salt, Sumisafe, Taien A, Taien H

Chemical Structure of Ammonium Polyphosphate:



***Note:** Data gaps for ammonium polyphosphate (CAS #6833-79-9) were addressed using the structurally similar chemical sodium tripolyphosphate (CAS #7758-29-4). The National Academy of Sciences selected sodium tripolyphosphate as a chemical surrogate for ammonium polyphosphate in the report “Toxicological Risks of Selected Flame-Retardant Chemicals (NAS 2000).”

For Polymers: Identify Monomers and Corresponding Properties

1. % of Each Monomer – n/a
2. Are the monomers blocked? – n/a
3. Molecular Weight (MW) of Polymer – ca 100,000 g/mol (Pinfa 2010).
4. % of Polymer with
 - a) MW <500 – n/a
 - b) MW <1,000 – n/a
5. % Weight Residual Monomers – n/a
6. Solubility/Dispersability/Swellability – ≤ 5 g/L (Clariant 2009)
7. Particle Size – approx. 15 μm (Clariant 1999)
8. Overall Polymer Charge – n/a

⁸ CPA recommends independent third-party validation of all Green Screen assessments. No independent third-party validation has been done for this assessment. Companies may not make marketing claims based on a Green Screen assessment that has not undergone an independent validation.

Identify Applications/Functional Uses: Flame retardant

Green Screen Rating⁹: Ammonium polyphosphate was assigned a Green Screen Benchmark Score of 4 based on low human toxicity and ecotoxicity.

Green Screen (Version 1) Levels of Concern for Ammonium Polyphosphate														
Human – Tier 1					Human – Tier 2				Eco		Fate		Physical	
C	M	R/D	ED	N	AT	Cr	Sn	ST	AA	CA	P	B	Ex	F
L	L	<i>L</i>	nd	nd	L	L	L	<i>L</i>	L	<i>L</i>	L	L	L	L

*Endpoints in italics were assigned using estimated values and professional judgment (Structure Activity Relationships)

Transformation Products and Ratings:

Identify relevant fate and transformation products (i.e., dissociation products, transformation products, valence states) and/or moieties of concern¹⁰

Life Cycle Stage	Transformation Pathway	Transformation Products	CAS #	Green Screen Rating
End of Life	Water hydrolysis	Ammonium phosphate	7783-28-0 (USAN) and 10124-31-9	Not present on the Red List of chemicals (CPA 2009).
End of Life	Combustion	Ammonia	7664-41-7	Not present on the Red List of chemicals (CPA 2009).
End of Life	Combustion	Phosphorous oxides	1314-56-3 and 14452-66-5	Not present on the Red List of chemicals (CPA 2009).
End of Life	Combustion	Nitrogen oxides	10102-43-9	Not present on the Red List of chemicals (CPA 2009).

*The above transformation products were screened against the CPA's table of Red List chemicals; none were found.

⁹ For inorganic chemicals with low human and ecotoxicity across all hazard endpoints and low bioaccumulation, persistence alone will not be deemed problematic. Inorganic chemicals that are only persistent will be evaluated under the criteria for Benchmark 4.

¹⁰ A moiety is a discrete chemical entity that is a constituent part or component of a substance. A moiety of concern is often the parent substance itself for organic compounds. For inorganic compounds, the moiety of concern is typically a dissociated component of the substance or a transformation product.

typhimurium tester strains TA 98, TA 100, TA 1535, TA 1537, and TA 1538, and *Escherichia coli* WP2uvrA with and without a metabolic activator at concentrations ranging from 4 to 5000 µg/plate in either a water or a DMSO vehicle (ESIS 2000).

Reproductive (R) and Developmental (D) Toxicity Score (H, M or L): L

Because no reproductive or developmental toxicity data were identified for APP, the structurally similar sodium tripolyphosphate was used as a surrogate. APP was assigned a score of Low based on analog data for sodium tripolyphosphate, which had no adverse effects on reproductive or developmental health.

Sodium tripolyphosphate

- Sodium tripolyphosphate had no effect on fertility, litter size, neonate growth, or neonate survival in a three generation reproduction study in rats administered 500 mg/kg-bw/day¹¹ sodium tripolyphosphate in their feed. No other details for this study were provided (NAS 2000).

Endocrine Disruption (ED) Score (H, M or L): nd

- APP is not listed as a potential endocrine disruptor on the EU Priority List of Suspected Endocrine Disruptors.
- APP is not listed as a potential endocrine disruptor on the OSPAR List of Chemicals of Possible Concern.
- APP is not listed as a potential endocrine disruptor on the Red List of Chemicals (CPA 2009).

Neurotoxicity (N) Score (H, M or L): nd

- APP is not classified as a developmental neurotoxicant (Grandjean and Landrigan 2006).
- APP is not listed as a potential neurotoxicant on the Red List of Chemicals (CPA 2009).

Human Health – Tier 2

Acute Mammalian (AT) Toxicity Score (H, M or L): L

APP was assigned a score of Low for acute mammalian toxicity based on oral and dermal LD₅₀ values greater than 2,000 mg/kg-bw. Data was from three different routes in two different species.

- *Oral*: An LD₅₀ of > 2,000 mg/kg-bw was identified in the rat (UNEP 2008).
- *Oral*: An LD₅₀ of 4,740 mg/kg-bw was identified in the rat (Clariant 2009).
- *Oral*: An LD₅₀ of > 2,000 mg/kg-bw was identified in the rabbit (UNEP 2008).
- *Inhalation*: An LC₅₀ of > 5.09 mg/L (4-hr exposure) was identified in the rat (UNEP 2008).

¹¹ The original report by Hodge (1964a) provides a concentration of 0.5% sodium tripolyphosphate administered to rats. The conversion to mg/kg-bw/day is as follows (assuming use of Fisher rat, as the strain is not provided in the study):

(5,000 mg sodium tripolyphosphate/kg chow * 0.018 kg chow/day)/0.180 kg-bw = 500 mg/kg-bw/day

- *Dermal*: An LD₅₀ of >5,000 mg/kg-bw was identified in the rat (UNEP 2008).
- *Dermal*: An LD₅₀ of >2,000 mg/kg-bw was identified in the rat (UNEP 2008).

Corrosion/ Irritation (Skin/ Eye) (Cr) Score (H, M or L): L

APP was assigned a score of Low for corrosion and irritation based on animal studies that showed the chemical to not be irritating to the skin or eyes of rabbits.

- *Dermal*: APP was not irritating to the skin of rabbits following a 4-hour occlusion in a Draize test. The test substance was 70% ammonium polyphosphate and 30% monoammonium phosphate. Additional details concerning this study were not provided (UNEP 2008).
- *Dermal*: APP was slightly irritating to the skin of rabbits following a 24-hour occlusive Patch test. Additional details concerning this study were not provided (ESIS 2000).
- *Dermal*: Exolit 456 (90% APP and 10% monoammonium phosphate) was not irritating in an OECD 404 “Acute Dermal irritation/corrosion” test. Additional details concerning this study were not provided (ESIS 2000).
- *Ocular*: APP was not irritating to the eyes of rabbits in a Draize test. The test substance was 70% ammonium polyphosphate and 30% monoammonium phosphate. Additional details concerning this study were not provided (ESIS 2000).
- *Ocular*: APP was not irritating to the eyes of rabbits. Additional details concerning this study were not provided (ESIS 2000).
- *Ocular*: Exolit 456 (90% APP and 10% melamine/formaldehyde) was not irritating to the eyes of rabbits following an OECD 405 “Acute Eye Irritation/Corrosion” test. Additional details concerning this study were not available (ESIS 2000).

Sensitization (Sn) Score (Skin and Respiratory) (H, M or L): L

APP was assigned a score of Low for sensitization because animal tests showed the chemical to be a poor sensitizing agent.

- *Dermal*: APP was found to be a poor skin-sensitizing agent in the Magnusson and Kligman maximization test. Twenty female guinea pigs were initially injected intradermally with a 25% (w/v) solution of APP. Topical induction was then attempted on day 7 with filter paper patches containing 75% (w/w) APP in distilled water. Only 1 of 20 animals had skin changes (scattered mild redness) at the application site 1 hour after removal of the patches. No animals had any visible skin reactions 24 hours after patch removal. None of the animals showed any tissue reaction either 24 or 48 hours after topical challenge with filter paper patches containing 50% or 75% solutions of APP. No other data was provided for this study (Safepharm 1993).

Systemic/ Organ (ST) Toxicity Score (includes organ effects and immunotoxicity) (H, M or L): L

Because no relevant systemic/organ toxicity data were identified for APP, the structurally similar sodium tripolyphosphate was used as a surrogate. APP was assigned a score of Low for systemic/organ toxicity based on analog data.

Sodium tripolyphosphate:

- Male and female rats (36/sex/dose) were administered 0, 3, and 5% sodium tripolyphosphate in their diets for 24 weeks. Nephrocalcinosis was observed at 3% dose level only. No other information was provided (JECFA 1974).

Ecotoxicity

Acute Aquatic (AA) Toxicity Score (H, M or L): L

APP was assigned a score of Low for acute aquatic toxicity based on LC₅₀ values of 100 mg/L or greater.

- APP has an LC₅₀ of > 101 mg/L in *Oncorhynchus mykiss* (freshwater fish, 96 hour) (UNEP 2008).
- APP has an LC₅₀ of 100 - 1,000 mg/L in *Danio rerio* (freshwater fish, 96 hour) (Clariant 2009).

Chronic Aquatic (CA) Toxicity Score (H, M or L): L

APP was assigned a Low for chronic aquatic toxicity based on professional opinion.

- APP has a molecular weight of 100,000 g/mol (Pinfa 2010). Insoluble polymers are not expected to be toxic to aquatic organisms unless the material is in the form of finely divided particles. Toxicity of these polymer particles does not depend on a specific structural feature, but occurs from occlusion of respiratory organs such as gills. For these polymers, toxicity occurs at high concentrations; >100 mg/L for acute toxicity and >10 mg/L for chronic toxicity (U.S. EPA 2010).

Environmental Fate

Persistence (P) Score (vH, H, M, or L): L

APP was assigned a score of Low for persistence based on a soil half-life less than 30 days and rapid biodegradation.

- APP breaks down into ammonia and phosphate rapidly in soil and sewage sludge (Leisewitz 2000).
- Hydrolysis of APP occurs very slowly in neutral solutions (UNEP 2008).
- The half-life of APP in soil ranged from 1.6 to 2.0 days under anaerobic conditions and from 5.3 to 8.7 days under aerobic conditions (UNEP 2008).
- Biodegradation tests are not applicable to APP because the methods are based on carbon oxidation and the ammonium present in APP may be nitrified (UNEP 2008).

Bioaccumulation (B) Score (vH, H, M, or L): L

APP was assigned a score of Low for bioaccumulation based on its insolubility.

- APP is not expected to bioaccumulate because it is an inorganic polymer (avg. MW = 100,000) and therefore insoluble in water (Pinfa 2010).

Physical Properties

Explosivity (Ex) Hazard Rating (H, M or L): L

APP was assigned a score of Low for explosivity because no basis for concern was identified.

- APP is not explosive- no other data provided (Clariant 2009).

Flammability (F) Hazard Rating (H, M or L): L

APP was assigned a score of Low for flammability because no basis for concern was identified.

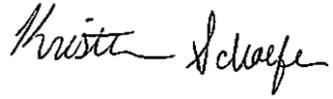
- APP is not flammable- no other data provided (Clariant 2009).

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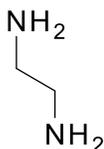
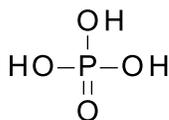


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**APPENDIX IX E: GREEN SCREEN FOR ETHYLENEDIAMINE PHOSPHATE
(CAS #14582-17-6)¹²**

Also Called: 1,2-Ethanediamine, phosphate, Ethylenediamine, salt with phosphoric acid

Chemical Structure of Ethylenediamine Phosphate:



***Note:** Data gaps for ethylene phosphate (CAS #14852-17-6) were addressed using the individual components of this mixture, ethylenediamine (CAS #107-15-3) and phosphoric acid (CAS #7664-38-2) as chemical surrogates.

For Inorganic Chemicals:

Define Form & Physiochemical Properties

4. Particle size (e.g. silica of respirable size) – n/a
5. Structure (e.g. amorphous vs. crystalline) – n/a
6. Mobility (e.g. Water solubility, volatility) – n/a

Identify Applications/Functional Uses: Flame retardant

Green Screen Rating¹³: Ethylenediamine phosphate was assigned a Green Screen Benchmark Score of 2 based on High chronic aquatic toxicity (CA), Moderate mutagenicity (M) and reproductive and developmental toxicity (R/D) (2d).

Green Screen (Version 1.0) Levels of Concern for Ethylenediamine Phosphate														
Human – Tier 1					Human – Tier 2				Eco		Fate		Physical	
C	M	R/D	ED	N	AT	Cr	Sn	ST	AA	CA	P	B	Ex	F
L	<i>M</i>	<i>M</i>	nd	nd	<i>M</i>	<i>H</i>	<i>H</i>	<i>M</i>	L	H	M	L	L	L

*Endpoints in italics were assigned using estimated values and professional judgment (Structure Activity Relationships).

¹² CPA recommends independent third-party validation of all Green Screen assessments. No independent third-party validation has been done for this assessment. Companies may not make marketing claims based on a Green Screen assessment that has not undergone an independent validation.

¹³ For inorganic chemicals with low human and ecotoxicity across all hazard endpoints and low bioaccumulation, persistence alone will not be deemed problematic. Inorganic chemicals that are only persistent will be evaluated under the criteria for Benchmark 4.

Transformation Products and Ratings:

Identify relevant fate and transformation products (i.e., dissociation products, transformation products, valence states) **and/or moieties of concern**¹⁴

Life Cycle Stage	Transformation Pathway	Transformation Products	CAS #	Green Screen Rating
End of life	Dissociation	Ethylenediamine	107-15-3	Present on the Red List of chemicals (CPA 2009).
End of life	Dissociation	Phosphoric acid	7664-38-2	Not present on the Red List of chemicals (CPA 2009).
End of life	Combustion	Carbon oxides	630-08-0 and 124-38-9	Present on the Red List of chemicals (CPA 2009).
End of Life	Combustion	Phosphorous oxides	1314-56-3 and 14452-66-5	Not present on the Red List of chemicals (CPA 2009).
End of Life	Combustion	Nitrogen oxides	10102-43-9	Not present on the Red List of chemicals (CPA 2009).

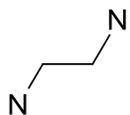
*The above transformation products were screened against the CPA's table of Red List chemicals.

Introduction

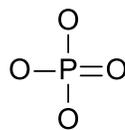
Ethylenediamine phosphate (CAS #14852-17-6) is a non-halogenated flame retardant composed of a mixture of ethylenediamine and phosphoric acid. No PEL, STEL or TLV have been established for ethylenediamine phosphate. Because there no relevant toxicity data were identified to assess possible skin/eye corrosion, skin/respiratory sensitization, mutagenicity, reproductive, developmental, acute or systemic toxicity of ethylenediamine phosphate, individual components of EDP were evaluated to address datagaps: ethylenediamine (CAS #107-15-3) and phosphoric acid (CAS #7664-38-2).

¹⁴ A moiety is a discrete chemical entity that is a constituent part or component of a substance. A moiety of concern is often the parent substance itself for organic compounds. For inorganic compounds, the moiety of concern is typically a dissociated component of the substance or a transformation product.

Chemical Structure of Surrogates:



Ethylenediamine (CAS #107-15-3)



Phosphoric acid (CAS #7664-38-2)

Human Health – Tier 1

Carcinogenicity (C) Score (H, M or L): L

Ethylenediamine phosphate was assigned a score of Low for carcinogenicity because no basis for concern was identified.

- Ethylenediamine phosphate is not listed as a known carcinogen by IARC, NTP, U.S. EPA, or CA Prop 65.

Mutagenicity (M) and Genotoxicity Score (H, M or L): M

Because no mutagenicity and genotoxicity data were identified for ethylenediamine phosphate, the components of the mixture were used as a surrogate. Ethylenediamine phosphate was assigned a score of Moderate for mutagenicity and genotoxicity based on conflicting results from several genotoxicity studies.

Ethylenediamine

- *In vitro* - An Ames Reverse Mutation assay was performed using *Salmonella typhimurium* tester strains TA100 and TA1535 in the presence and absence of metabolic activation at concentrations ranging from 0-6667 µg/plate and determined to be positive for mutagenicity (UNEP 2001).
- *In vitro* - An Ames Reverse Mutation assay was performed using *Salmonella typhimurium* tester strains TA98 and TA1537 in the presence and absence of metabolic activation at concentrations ranging from 0-3333 µg/plate and determined to be negative for mutagenicity (UNEP 2001).
- *In vitro* - An Ames Reverse Mutation assay was performed using *Salmonella typhimurium* tester strains TA98, TA100, TA 1535, TA 1537 and TA1538 in the presence and absence of metabolic activation at concentrations ranging from 90-9000 µg/plate and determined to be negative for mutagenicity (UNEP 2001).
- *In vitro* - An Ames Reverse Mutation assay was performed using *Salmonella typhimurium* tester strains TA98, TA100, TA 1535, and TA 1537 in the presence and absence of metabolic activation at concentrations ranging from 0-5000 µg/plate. Mutagenicity was ambiguous in TA 100 with metabolic activation, and negative in all other strains (UNEP 2001).
- *In vitro* – An HGPRT assay was performed using Chinese hamster ovary cells in the presence and absence of metabolic activation at concentrations ranging from 0-897 µg/plate and found to be negative for mutagenicity (UNEP 2001).
- *In vitro* – A sister chromatid exchange assay was performed using Chinese hamster ovary cells in the presence and absence of metabolic activation at concentrations ranging from 0-448 µg/plate and found to be negative for mutagenicity (UNEP 2001).

Phosphoric acid

- *In vitro* - An Ames Reverse Mutation assay was performed using *Salmonella typhimurium* tester strains TA97, TA98, TA100, and TA104 in the presence and absence of metabolic activation at concentrations ranging from 917-3668 µg/plate and determined to be negative for mutagenicity (CCRIS 2010).
- *In vitro* - An Ames Reverse Mutation assay was performed using *Salmonella typhimurium* tester strains in the presence and absence of metabolic activation and determined to be negative for mutagenicity. Strains and concentrations were not reported (ESIS 2000).

Reproductive (R) and Developmental (D) Toxicity Score (H, M or L): M

Because no reproductive and developmental toxicity data were identified for ethylenediamine phosphate, the components of the mixture were used as a surrogate. Ethylenediamine phosphate was assigned a score of Moderate for reproductive and developmental toxicity based on animal studies for ethylenediamine.

Ethylenediamine

- A 2-generation reproductive study was conducted on F344 rats (13 male and 26 female/dose level). Ethylenediamine was administered at concentrations of 50, 150, and 500 mg/kg by oral feeding daily starting 100 days prior to mating of F₀ until weaning of F₂ rats. Significant reduction in parental body weight gain was observed in the 150 and 500 mg/kg groups of male and female rats. A higher incidence of hepatocellular pleomorphism in both sexes of the 500 mg/kg group was observed and a significant decrease in the prevalence of kidney tubular mineralization in female rats at 150 mg/kg. No evidence of fertility impairment or embryotoxic effects was observed. A parental NOAEL of 50 mg/kg and a F₁ offspring NOAEL of 150 mg/kg were reported by the authors (UNEP 2001).
- A development toxicity study was performed on New Zealand White rabbits (26/dose). Rabbits were administered 0, 10, 40, and 80 mg/kg of ethylenediamine (purity not reported) on gestation days six through nineteen. No significant effects were observed on maternal food intake, body weight gain, liver or kidney weight, or uterine weight. No effects were observed on viability, litter size, fetal weight or fetal morphology. A NOAEL of > 80 mg/kg for maternal and fetal toxicity was reported by the authors (UNEP 2001).

Phosphoric acid

- A 1-generation reproductive study was conducted on rats (strain/sex/number not reported). Phosphoric acid was administered at concentrations of 180 and 375 mg/kg by oral feeding for 29 weeks. No harmful effects on the growth of the offspring or parental rats were reported at the highest concentration (ESIS 2000).

Endocrine Disruption (ED) Score (H, M or L): nd

- Ethylenediamine phosphate is not listed as a potential endocrine disruptor on the EU Priority List of Suspected Endocrine Disruptors.
- Ethylenediamine phosphate is not listed as a potential endocrine disruptor on the OSPAR List of Chemicals of Possible Concern.
- Ethylenediamine phosphate is not listed as a potential endocrine disruptor on the Red List of Chemicals (CPA 2009).

Neurotoxicity (N) Score (H, M or L): nd

- Ethylenediamine phosphate is not classified as a developmental neurotoxicant (Grandjean and Landrigan 2006).
- Ethylenediamine phosphate is not listed as a potential neurotoxicant on the Red List of Chemicals (CPA 2009).

Human Health – Tier 2**Acute Mammalian (AT) Toxicity Score (H, M or L): M**

Because no acute mammalian toxicity data were identified for ethylenediamine phosphate, the components of the mixture were used as a surrogate. A score of Moderate for acute mammalian toxicity was assigned to ethylenediamine phosphate based on oral LD₅₀ values between 50 and 2,000 mg/kg-bw and dermal LD₅₀ values between 200 and 2,000 mg/kg-bw. Data is from two surrogates using three different routes in three different species.

Ethylenediamine

- *Oral*: LD₅₀ (rat) = 637 mg/kg (UNEP 2001).
- *Oral*: LD₅₀ (rat) = 1850 mg/kg (UNEP 2001).
- *Oral*: LD₅₀ (rat) = 1050 mg/kg (UNEP 2001).
- *Oral*: LD₅₀ (rat) = 1500 mg/kg (UNEP 2001).
- *Oral*: LD₅₀ (mouse) = 1000 mg/kg (ChemIDPlus 2010).
- *Dermal*: LD₅₀ (rabbit) = 560 mg/kg (UNEP 2001).
- *Dermal*: LD₅₀ (rat) = 1000 mg/kg (UNEP 2001).
- *Inhalation*: LC₅₀ (rat) = 29 mg/L (ChemIDPlus 2010).

Phosphoric acid

- *Oral*: LD₅₀ (rat) = 1530 mg/kg (ESIS 2000).
- *Dermal*: LD₅₀ (rabbit) = 2740 mg/kg (ESIS 2000).
- *Inhalation*: LC₅₀ (rabbit) = 1.689 mg/L (ESIS 2000).

Corrosion/ Irritation (Skin/ Eye) (Cr) Score (H, M or L): H

Because no corrosion/irritation toxicity data were identified for ethylenediamine phosphate, the components of the mixture were used as a surrogate. Ethylenediamine phosphate was assigned a score of High for corrosion and irritation based on animal studies showing the chemical to be corrosive and irritating.

Ethylenediamine

- *Dermal*: Application of an aqueous solution of 70% ethylenediamine to the skin of rabbits (# not reported) caused complete destruction within 6 to 12 minutes. A 10% solution of ethylenediamine in water caused a burn within 24 hours. A dermal NOEL of 0.1% was reported by the authors (UNEP 2001).
- *Ocular*: A 10% solution in water caused moderate corneal damage and extensive conjunctivitis. A 1% solution was essentially non-irritating. Species and number of animals tested were not reported (UNEP 2001).
- *Ocular*: Vapors ethylenediamine are mildly irritating to the eye after 10 seconds at 200 ppm while 400 ppm is intolerable. Species and number of test subjects were not reported (UNEP 2001).

Phosphoric acid

- *Dermal*: Several dermal studies have been completed on the compound. Phosphoric has been classified as irritating and corrosive at concentrations ranging from 35 to 100% (ESIS 2000)
- *Ocular*: Phosphoric acid was found to be not irritating to the eyes of rabbits following OECD guideline 405 at concentrations of 10 and 17% phosphoric acid (ESIS 2000).
- *Ocular*: Phosphoric acid is classified as potentially irritating to the eyes of humans (ESIS 2000).

Sensitization (Sn) Score (Skin and Respiratory) (H, M or L): H

Because no sensitization data were identified for ethylenediamine phosphate, the components of the mixture were used as a surrogate. Ethylenediamine phosphate was assigned a score of High for sensitization based on ethylenediamine testing positive for skin sensitization.

Ethylenediamine

- *Dermal*: Several skin sensitization studies have been reported for ethylenediamine including the following: guinea pig maximization test, draize test, repeated insult patch test, single injection adjuvant test, mouse optimization test, and a mouse ear swelling test. The test substance was confirmed to be sensitizing in the reported studies (UNEP 2001).
- *Respiratory/Dermal*: Ethylenediamine is associated with risk phrase 42/43. May cause sensitization by inhalation and skin contact (EINECS 2010).

Phosphoric acid

- *Dermal*: Phosphoric acid is classified as not sensitizing to humans. No other data was available for this study (ESIS 2000).

Systemic/ Organ (ST) Toxicity Score (includes organ effects and immunotoxicity) (H, M or L): M

Because no systemic/organ toxicity data were identified for ethylenediamine phosphate, the components of the mixture were used as a surrogate. Ethylenediamine phosphate was assigned a score of Moderate for systemic/organ toxicity based on repeat-dose analog studies suggesting renal toxicity in rodents.

Ethylenediamine

- A 13 week repeat dose oral toxicity study was conducted on F344 rats (10/sex/group). Concentrations of 0, 100, 200, 400, 600, and 800 mg/kg of ethylenediamine (purity not reported) were administered daily (5 days/week) by oral gavage for 13 weeks. Body weight gains were decreased in male and female rats administered 200 to 800 mg/kg. Several females in the 600 mg/kg and higher groups appeared to have smaller uterine horns and the 800 mg/kg group had smaller ovaries. Renal tubular lesions were noted in the 600 and 800 mg/kg groups. Male and female rats also exhibited bilateral cataracts in the 600 mg/kg group after 12 weeks. A LOAEL of 100 mg/kg was reported by the authors. This test study was reported to have followed OECD guideline 408 “Subchronic Oral Toxicity – Rodent: 90-day Study” (UNEP 2001).
- A 13 week repeat dose oral toxicity study was conducted on B6C3F1 mice (10/sex/group). Concentrations of 0, 25, 50, 100, 200, and 400 mg/kg of

ethylenediamine (purity not reported) were administered daily (5 days/week) by oral gavage for 13 weeks. No body weight changes were observed. There were no treatment related gross lesions. Histopathologic changes were noted in the kidneys at 499 mg/kg. The kidney lesion was characterized by mild to moderate degeneration of the renal tubular epithelium. A NOEL of 200 mg/kg was reported by the authors. This test study was reported to have followed OECD guideline 408 “Subchronic Oral Toxicity – Rodent: 90-day Study” (UNEP 2001).

Phosphoric acid

- No relevant data were identified for this phosphoric acid.

Ecotoxicity

Acute Aquatic (AA) Toxicity Score (H, M or L): L

Ethylenediamine phosphate was assigned a score of Low for acute aquatic toxicity based on LC₅₀ values greater than 100 mg/L.

- An LC₅₀ of > 100 mg/L was identified in fish (fish, 96 hour) (Fisk et al. 2003).
- ECOSAR – Ethylenediamine phosphate is designated to the aliphatic amines and neutral organics ECOSAR classes. The estimated L/EC₅₀ values are 6266.691 mg/L (daphnid, 48 hr), and 320.865 mg/L (algae, 96 hr) (U.S. EPA 2009).

Chronic Aquatic (CA) Toxicity Score (H, M or L): H

Ethylenediamine phosphate was assigned a score of High for chronic aquatic toxicity based on an NOEC value < 0.1 mg/L.

- ECOSAR – The estimated ChV values are 2375.747 mg/L (fish, 96 hr), 0.082 mg/L (daphnid, 48 hr), and 723.378 mg/L (algae, 96 hr) (U.S. EPA 2009).

Environmental Fate

Persistence (P) Score (vH, H, M, or L): M

Ethylenediamine phosphate was assigned a score of Moderate for persistence based on a soil half life of 30 days and water half life of 15 days.

- EPI Suite – BIOWIN model results indicate ethylenediamine phosphate is not readily biodegrade, and has a predicted degradation time of weeks. STP removal expected using BIOWIN/EPA Draft Method results indicate 75.06% total removal, with 74.44% due to biodegradation. Fugacity III modeling predicts 67.1% partitioning to soil with a half-life of 30 days, and 32.9% partitioning to water with a half-life of 15 days (U.S. EPA 2010).

Bioaccumulation (B) Score (vH, H, M, or L): L

Ethylenediamine phosphate was assigned a score of Low for bioaccumulation based on a BCF value less than 100.

- BCFBAF predicts a bioconcentration factor (BCF) of 3.162 L/kg wet-wt and a log K_{ow} of -4.54 (U.S. EPA 2010). BCF is used in instances where log K_{ow} is <5.

Physical Properties

Explosivity (Ex) Hazard Rating (H, M or L): L

Because no explosivity data were identified for ethylenediamine phosphate, the components of the mixture were used as a surrogate. Ethylenediamine phosphate was assigned a score of Low for explosivity because no basis for concern was identified.

Ethylenediamine

- Ethylenediamine is stable (ScienceLab 2008).

Phosphoric acid

- Phosphoric acid is not explosive (ESIS 2000).

Flammability (F) Hazard Rating (H, M or L): L

Because no flammability data were identified for ethylenediamine phosphate, the components of the mixture were used as a surrogate. Ethylenediamine phosphate was assigned a score of Low for explosivity because no basis for concern was identified.

Ethylenediamine

- Ethylenediamine is flammable (ScienceLab 2008).

Phosphoric acid

- Phosphoric acid is not flammable (ESIS 2000).

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EPI Suite Results for Ethylenediamine Phosphate:

CAS Number: 14852-17-6
SMILES : NCCN(H)(H)(H)OP(=O)(O)O
CHEM : 1,2-Ethanediamine, phosphate
MOL FOR: C2 H11 N2 O4 P1
MOL WT : 158.10

----- EPI SUMMARY (v4.00) -----

Physical Property Inputs:

Log Kow (octanol-water): -----
Boiling Point (deg C) : -----
Melting Point (deg C) : -----
Vapor Pressure (mm Hg) : -----
Water Solubility (mg/L): -----
Henry LC (atm-m³/mole) : -----

Log Octanol-Water Partition Coef (SRC):

Log Kow (KOWWIN v1.67 estimate) = -4.54

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPVP v1.43):

Boiling Pt (deg C): 480.00 (Adapted Stein & Brown method)
Melting Pt (deg C): 90.27 (Mean or Weighted MP)
VP(mm Hg,25 deg C): 6.06E-011 (Modified Grain method)
VP (Pa, 25 deg C) : 8.07E-009 (Modified Grain method)
Subcooled liquid VP: 2.58E-010 mm Hg (25 deg C, Mod-Grain method)
: 3.44E-008 Pa (25 deg C, Mod-Grain method)

Water Solubility Estimate from Log Kow (WSKOW v1.41):

Water Solubility at 25 deg C (mg/L): 1e+006
log Kow used: -4.54 (estimated)
no-melting pt equation used

Water Sol Estimate from Fragments:

Wat Sol (v1.01 est) = 1e+006 mg/L

ECOSAR Class Program (ECOSAR v1.00):

Class(es) found:
Aliphatic Amines

Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:

Bond Method : 9.03E-027 atm-m³/mole (9.15E-022 Pa-m³/mole)
Group Method: Incomplete

For Henry LC Comparison Purposes:

User-Entered Henry LC: not entered
Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
HLC: 1.261E-017 atm-m³/mole (1.277E-012 Pa-m³/mole)
VP: 6.06E-011 mm Hg (source: MPBPVP)
WS: 1E+006 mg/L (source: WSKOWWIN)

Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1.10]:

Log Kow used: -4.54 (KowWin est)
Log Kaw used: -24.433 (HenryWin est)
Log Koa (KOAWIN v1.10 estimate): 19.893
Log Koa (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10):

Biowin1 (Linear Model) : 0.8261
Biowin2 (Non-Linear Model) : 0.8669

Expert Survey Biodegradation Results:

Biowin3 (Ultimate Survey Model): 2.8742 (weeks)
Biowin4 (Primary Survey Model) : 3.6629 (days-weeks)

MITI Biodegradation Probability:

Biowin5 (MITI Linear Model) : 0.3647
Biowin6 (MITI Non-Linear Model): 0.2299

Anaerobic Biodegradation Probability:

Biowin7 (Anaerobic Linear Model): 0.6277

Ready Biodegradability Prediction: NO

Hydrocarbon Biodegradation (BioHCwin v1.01):

Structure incompatible with current estimation method!

Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:

Vapor pressure (liquid/subcooled): 3.44E-008 Pa (2.58E-010 mm Hg)

Log Koa (Koawin est): 19.893

Kp (particle/gas partition coef. (m3/ug)):

Mackay model : 87.2
Octanol/air (Koa) model: 1.92E+007

Fraction sorbed to airborne particulates (phi):

Junge-Pankow model : 1
Mackay model : 1
Octanol/air (Koa) model: 1

Atmospheric Oxidation (25 deg C) [AopWin v1.92]:

Hydroxyl Radicals Reaction:

OVERALL OH Rate Constant = 42.6481 E-12 cm³/molecule-sec
Half-Life = 0.251 Days (12-hr day; 1.5E6 OH/cm³)
Half-Life = 3.010 Hrs

Ozone Reaction:

No Ozone Reaction Estimation

Fraction sorbed to airborne particulates (phi):

1 (Junge-Pankow, Mackay avg)
1 (Koa method)

Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (KOCWIN v2.00):

Koc : 6.269 L/kg (MCI method)
Log Koc: 0.797 (MCI method)
Koc : 0.02976 L/kg (Kow method)
Log Koc: -1.526 (Kow method)

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v2.00]:

Rate constants can NOT be estimated for this structure!

Bioaccumulation Estimates (BCFBAF v3.00):

Log BCF from regression-based method = 0.500 (BCF = 3.162 L/kg wet-wt)
Log Biotransformation Half-life (HL) = -2.8838 days (HL = 0.001307 days)
Log BCF Arnot-Gobas method (upper trophic) = -0.049 (BCF = 0.893)
Log BAF Arnot-Gobas method (upper trophic) = -0.049 (BAF = 0.893)
Kow log used: -4.54 (estimated)

Volatilization from Water:

Henry LC: 9.03E-027 atm-m³/mole (estimated by Bond SAR Method)
 Half-Life from Model River: 8.153E+022 hours (3.397E+021 days)
 Half-Life from Model Lake : 8.894E+023 hours (3.706E+022 days)

Removal In Wastewater Treatment:

Total removal: 1.85 percent
 Total biodegradation: 0.09 percent
 Total sludge adsorption: 1.75 percent
 Total to Air: 0.00 percent
 (using 10000 hr Bio P,A,S)

Removal In Wastewater Treatment:

Total removal: 75.06 percent
 Total biodegradation: 74.44 percent
 Total sludge adsorption: 0.62 percent
 Total to Air: 0.00 percent
 (using Biowin/EPA draft method)

Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	6.65e-016	6.02	1000
Water	32.9	360	1000
Soil	67.1	720	1000
Sediment	0.0688	3.24e+003	0

Persistence Time: 622 hr

ECOSAR Results for Ethylenediamine Phosphate:

SMILES : NCCN(H)(H)(H)OP(=O)(O)O
 CHEM : 1,2-Ethanediamine, phosphate
 CAS Num: 014852-17-6
 ChemID1:
 ChemID2:
 ChemID3:
 MOL FOR: C2 H11 N2 O4 P1
 MOL WT : 158.10
 Log Kow: -4.54 (KowWin estimate)
 Melt Pt:
 Wat Sol: 1E+006 mg/L (WskowWin estimate)

ECOSAR v1.00 Class(es) Found

 Aliphatic Amines

ECOSAR Class	Organism	Predicted		
		Duration	End Pt	mg/L (ppm)
Aliphatic Amines	: Fish	96-hr	LC50	2.4e+005
Aliphatic Amines	: Daphnid	48-hr	LC50	6266.691
Aliphatic Amines	: Green Algae	96-hr	EC50	320.865
Aliphatic Amines	: Fish		ChV	2375.747
Aliphatic Amines	: Daphnid		ChV	0.082
Aliphatic Amines	: Green Algae		ChV	723.378
Aliphatic Amines	: Fish (SW)	96-hr	LC50	2.42e+005
Aliphatic Amines	: Mysid Shrimp (SW)	96-hr	LC50	6979.869
Aliphatic Amines	: Green Algae (SW)	96-hr	EC50	322.587

Aliphatic Amines	: Fish (SW)	ChV	2375.747
Aliphatic Amines	: Mysid Shrimp (SW)	ChV	0.082
Aliphatic Amines	: Green Algae (SW)	ChV	564.342

Neutral Organic SAR	: Fish	96-hr	LC50	4.2e+007 *
(Baseline Toxicity)	: Daphnid	48-hr	LC50	1.1e+007 *
	: Green Algae	96-hr	EC50	3.23e+005
	: Fish	ChV		4.6e+006 *
	: Daphnid	ChV		3.19e+005
	: Green Algae	ChV		35379.375

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect.

Aliphatic Amines:

For Fish 96-hr LC50: For aliphatic amines with log Kow greater than 7.0, a test duration of greater than 96 hrs may be required for proper expression of toxicity. Also, if the toxicity value obtained by the use of this equation exceeds the water solubility (measured or estimated), mortalities greater than 50% would not be expected in a saturated solution during an exposure period of 96 hrs.

For Daphnid 48-hr LC50: For aliphatic amines with log Kow greater than 5.0, a test duration of greater than 48 hrs may be required for proper expression of toxicity. Also, if the toxicity value obtained by the use of this equation exceeds the water solubility (measured or estimated), significant mortalities would not be expected in a saturated solution during an exposure period of 48 hrs.

For Green Algae Acute Toxicity Values: If the log Kow of the chemical is greater than 7, or if the compound is solid and the EC50 exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

For Mysid Shrimp Acute Toxicity Values: If the log Kow of the chemical is greater than 6, or if the compound is solid and the EC50 exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

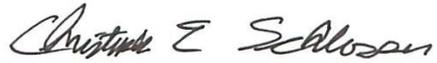
For Fish and Daphnid Chronic Toxicity Values: If the log Kow of the chemical is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

For Green Algae Chronic Toxicity Values: If the log Kow of the chemical is greater than 7.0, or if the compound is solid and the ChV exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

ECOSAR v1.00 SAR Limitations:

Maximum LogKow: 6.0 (Fish, Mysid LC50)
Maximum LogKow: 5.0 (Daphnid LC50)
Maximum LogKow: 7.0 (Green Algae EC50)
Maximum LogKow: 8.0 (Fish, Daphnid ChV)
Maximum LogKow: 7.0 (Green Algae ChV)
Maximum Mol Wt: 1000
Baseline Toxicity SAR Limitations:-----
Maximum LogKow: 5.0 (Fish 96-hr LC50; Daphnid LC50)
Maximum LogKow: 6.4 (Green Algae EC50)
Maximum LogKow: 8.0 (ChV)
Maximum Mol Wt: 1000

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APPENDIX IX F: GREEN SCREEN FOR MAGNESIUM HYDROXIDE (CAS #1309-42-8)¹⁵

Also Called: 200-06H, Alcanex NHC 25, Asahi Glass 200-06, Baschem 12, CCRIS 3342, Combustrol 500, DP 393, DSB 100, Duhor, Duhor N, EINECS 215-170-3, Ebson RF, FloMag H, FloMag HUS, HSDB 659, Hydro-mag MA, Hydrofy G 1.5, Hydrofy G 2.5, Hydrofy N, KX 8S(A), KX 8S(B), Ki 22-5B, Kisuma 4AF, Kisuma 5, Kisuma 5A, Kisuma 5B, Kisuma 5B-N, Kisuma 5BG, Kisuma 5E, Kisuma 78, Kisuma S 4, Kyowamag F, Lycal 96 HSE, Mag Chem MH 10, Magnesia hydrate, MagneClear 58, Magnesia magma, Magnesia, [milk of], Magnesiumaito, Magnesium dihydroxide, Magnesium hydroxide, Magnesium hydroxide (Mg(OH)₂), Magnesium hydroxide gel, Magnesium oxide (Mg(OH)₂), Magnesium(II) hydroxide, Magnifin H 10, Magox, Marinc H, Marinc H 1241, Martinal VPF 8812, Milk of magnesia, Milmag, Mint-O-Mag, Nermalite, Oxaine M, Phillips Magnesia Tablets, Phillips Milk of Magnesia Liquid, Reachim, S/G 84, Star 200, UNII-NBZ3QY004S, Versamag

Chemical Structure of Magnesium Hydroxide:



***Note:** Data gaps for this chemical were addressed by using other structurally similar magnesium salts such as magnesium chloride, magnesium lactate, and magnesium citrate. These chemicals in particular were selected due to the fact they are expected to dissociate in stomach acid and because they have been used in other risk assessments as surrogates for magnesium hydroxide (NAS 2000, U.S. EPA 2008).

For Inorganic Chemicals:

Define Form & Physiochemical Properties

7. Particle size (e.g. silica of respirable size) – n/a
8. Structure (e.g. amorphous vs. crystalline) – n/a
9. Mobility (e.g. Water solubility, volatility) – 0.009 g/L at 18°C (Hodgman 1959); 0.04 g/L at 100°C (Hodgman 1959)

Identify Applications/Functional Uses: Flame retardant

Green Screen Rating¹⁶: Magnesium hydroxide was assigned a Benchmark Score of 2 based on a very High persistence (P) rating and a Moderate corrosion (Cr) rating (2c).

Green Screen (Version 1.0) Levels of Concern for Magnesium Hydroxide														
Human – Tier 1					Human – Tier 2				Eco		Fate		Physical	
C	M	R/D	ED	N	AT	Cr	Sn	ST	AA	CA	P	B	Ex	F
L	L	L	nd	<i>L</i>	L	M	<i>L</i>	M	L	L	vH	L	L	L

*Endpoints in italics were assigned using estimated values and professional judgment (Structure Activity Relationships).

¹⁵ CPA recommends independent third-party validation of all Green Screen assessments. No independent third-party validation has been done for this assessment. Companies may not make marketing claims based on a Green Screen assessment that has not undergone an independent validation.

¹⁶ For inorganic chemicals with low human and ecotoxicity across all hazard endpoints and low bioaccumulation, persistence alone will not be deemed problematic. Inorganic chemicals that are only persistent will be evaluated under the criteria for Benchmark 4.

Transformation Products and Ratings:

Identify relevant fate and transformation products (i.e., dissociation products, transformation products, valence states) and/or moieties of concern¹⁷

Life Cycle Stage	Transformation Pathway	Transformation Products	CAS #	Green Screen Rating
End of Life	Hydrolysis	Water	7732-18-5	4
End of Life	Hydrolysis	Magnesium	7439-95-4	Not present on the Red List of Chemicals (CPA 2009)
End of Life	Hydrolysis	Hydrogen peroxide	7722-84-1	Not present on the Red List of Chemicals (CPA 2009)

*The above transformation products were screened against the CPA's table of Red List chemicals; none were found.

Introduction

Magnesium hydroxide is commonly used as an antacid and is the active ingredient in the laxative, milk of magnesia (NAS 2000). Additionally, it is used as a residual fuel-oil additive, an alkali drying agent in food, a color-retention agent, and is an ingredient of tooth (NAS 2000). $Mg(OH)_2$ is used as a flame retardant (FR) in commercial furniture applications in the United States and in commercial and residential furniture in the United Kingdom (Fire Retardant Chemicals Association 1998). The stability of $Mg(OH)_2$ at temperatures above 300°C allows it to be incorporated into several polymers (IPCS 1997).

Human Health – Tier 1

Carcinogenicity (C) Score (H, M or L): L

Magnesium hydroxide was assigned a score of Low for carcinogenicity due to findings from several animal studies.

- Not listed as a known carcinogen by IARC, NTP, U.S. EPA, or CA Prop 65.
- Oncologic results predict the hazard rating for carcinogenicity for magnesium hydroxide to be low (OncoLogic 2005).
- The incidence of all cancers among 2,391 Norwegian males who worked between 1951 and 1974 in a factory producing magnesium metal was not significantly increased when compared with cancer incidence for the Norwegian nation population of the same age. The number of cases of lip as well as stomach and lung cancers was significantly increased. Workers in this study were also

¹⁷ A moiety is a discrete chemical entity that is a constituent part or component of a substance. A moiety of concern is often the parent substance itself for organic compounds. For inorganic compounds, the moiety of concern is typically a dissociated component of the substance or a transformation product.

exposed to magnesium oxide dust, coal dust, chlorine gas, hydrochlorine aerosols, chlorinated aromatics, and sulphur dioxide. Therefore, it is not possible to determine whether exposure to magnesium dust alone is responsible for the observed elevations in cancer incidence (Heldaas 1989).

- Exposure of male Wistar rats to short (4.9x0.31 mm) or long (12x0.44) MgSO₄·3H₂O filaments by inhalation (6 hours per day, 5 days per week for 1 year) was not associated with an increase in the incidence of any tumor types in animals sacrificed 1 day or 1 year after cessation of exposure. One year after exposure, one pulmonary adenoma was observed in animals that had been exposed to long filaments for 3 weeks and none in controls. One year after exposure, neoplastic lesions were observed in control animals and short- and long-filament treated rats that had been exposed for 1 year. Two pulmonary adenomas were observed in the exposed animals and one in control animals. No hepatocellular adenomas or carcinomas occurred in controls, one hepatocellular adenoma was found in the long-filament group, and one hepatocellular carcinoma was found in the short-filament group, respectively (Hori 1994).
- Mice fed 0.5% or 2% of aqueous MgCl₂ in their diet for 96 weeks (68, or 336 mg/kg-day for males; 87 or 470 mg/kg-day for females) showed no significant change in the incidence of malignant lymphoma and leukemia. Dose-related increases in incidence of malignant lymphoma and leukemia occurred in male mice (controls, five of 50; low dose, seven of 50; high dose, eleven of 50), but not in females (controls, nine of 49; low dose, 17 of 50; high dose, 11 of 50). The incidence of hepatocellular carcinomas in male mice was decreased in a dose-related manner (controls, 13 of 50; low dose, six of 50; high dose, four of 50) and the incidence in high-dose males was significantly different from that in controls. Toxicity in female mice (i.e., decreased body weight) suggests that the study was conducted at or near the maximum tolerated dose (MTD) for females (Kurata 1989).
- Several studies in rats have shown that dietary Mg(OH)₂ can protect against chemically induced bowel carcinogenesis by suppressing hyperproliferation of the colon epithelium. Dietary levels of 250 ppm Mg(OH)₂ inhibited the incidence of colon adenoma and adenocarcinoma in rats given carcinogens methylazoxymethanol acetate (MAM acetate) or 1, 2-dimethylhydrazine (Tanaka 1989; Morishita 1991; Mori 1993). Administration of Mg(OH)₂ in the diet and the bowel carcinogen cholic acid reduced cell proliferation in bowel tissue (Wang 1993). Dietary Mg(OH)₂ also prevented the expression of *c-myc* gene in colon mucosa cells of MAM acetate-treated rats (Wang 1993).
- The subcommittee concludes that Mg(OH)₂ is not likely to be carcinogenic to humans by the oral route. No adequate data are available to assess the carcinogenicity of Mg(OH)₂ by the dermal or inhalation or routes of exposure (NAS 2000).

Mutagenicity (M) and Genotoxicity Score (H, M or L): L

Magnesium hydroxide was assigned a score of Low for mutagenicity based on negative results from several genotoxicity assays.

- MgCl₂ was judged to be a non-mutagen in the Ames assay when tested with and without metabolic activation and it did not induce chromosomal aberrations in

Chinese hamster fibroblast cells in vitro (Ishidate 1984). Chromatid gaps, breaks, and exchanges were observed in Chinese hamster lung fibroblasts treated with $MgCl_2$ at concentrations of 8.0 and 12.0 mg/ml but not at or below concentrations of 4 mg/mL (Ashby and Ishidate 1986). Since positive results occurred at only high concentrations, the authors suggest that the clastogenic effects observed may be an artifact induced by hypertonic solutions. $MgCl_2$ did not induce mutations in mouse lymphoma L5178/TK+/- cells at concentrations of 5.7–18.1 mg Mg^{2+} /ml (Amacher and Paillet 1980). $MgSO_4$ was not mutagenic in *Salmonella typhimurium* (strains TA100, TA1535) and *Escherichia coli* WP2 uvrA at concentrations of 313–5,000 mg/plate (Oguma 1998). $MgSO_4$ was not mutagenic in *Salmonella* strain TA98 tested without metabolic activation and strain TA1537 tested with metabolic activation at a concentration of 156–5,000 mg/plate (Oguma 1998).

Reproductive (R) and Developmental (D) Toxicity Score (H, M or L): L

Magnesium hydroxide was assigned a score of Low for reproductive and developmental toxicity based on the results from one animal study and one study in humans.

- No maternal or reproductive effects were observed in a 10 day (GD 6-15) oral reproductive/developmental study on rats using $MgCl_2$. The authors of the study determined the NOAEL to be >96 mg/kg/day for Mg^{2+} (NAS 2000).
- A repeated dose/developmental (3rd trimester) study on humans produced no effect on newborns except slightly increased body weight and hypermagnesiumemia. Cord serum magnesium levels reported to be 70-100% of maternal levels (potentially causing neurological depression in neonate, characterized by respiratory depression, muscle weakness, decreased reflexes). Prolonged magnesium treatment during pregnancy may be associated with maternal and fetal hypocalcemia and adverse effects on fetal bone mineralization (HSDB 2003).

Endocrine Disruption (ED) Score (H, M or L): nd

- Not listed as a potential endocrine disruptor on the EU Priority List of Suspected Endocrine Disruptors.
- Not listed as a potential endocrine disruptor on the OSPAR List of Chemicals of Possible Concern.
- Not listed as a potential endocrine disruptor on the Red List of Chemicals (CPA 2009).
- No other relevant endocrine disruption data could be identified for magnesium hydroxide.

Neurotoxicity (N) Score (H, M or L): L

Magnesium hydroxide was assigned a score of Low for neurotoxicity based on professional judgement.

- Not classified as a developmental neurotoxicant (Grandjean and Landrigan 2006).
- Not listed as a potential neurotoxicant on the Red List of Chemicals (CPA 2009).
- Magnesium hydroxide is expected to be of low hazard for neurotoxicity based on professional judgment (U.S. EPA 2008).

Human Health – Tier 2

Acute Mammalian (AT) Toxicity Score (H, M or L): L

Magnesium hydroxide was assigned a score of Low for acute mammalian toxicity based on oral LD₅₀ values greater than 2,000 mg/kg-bw. This score is based on data from one route of exposure in two different species of animals.

- *Oral*: An LD₅₀ of 8,500 mg/kg was determined in the rat (Lewis 2000).
- *Oral*: An LD₅₀ of 8,500 mg/kg was determined in the mouse (Lewis 2000)

Corrosion/Irritation (Skin/ Eye) (Cr) Score (H, M or L): M

Magnesium hydroxide was assigned a score of Moderate for corrosion/irritation based on the substance being moderately irritating to the eyes of rabbits.

- *Dermal*: No relevant data were identified for magnesium hydroxide.
- *Ocular*: Moderately irritating to rabbit eyes (IUCLID 2000).
- *Ocular*: Administration of milk of magnesia twice a day for 3-4 days caused damage to corneal epithelium of rabbit eyes; however, effects disappeared within 2-3 days. No additional details were provided (HSDB 2003).

Sensitization (Sn) Score (Skin and Respiratory) (H, M or L): L

Magnesium hydroxide was assigned a score of Low for sensitization based on professional judgment.

- Magnesium hydroxide is not expected to cause skin sensitization based on professional judgment. No other details were provided (U.S. EPA 2008).

Systemic/ Organ (ST) Toxicity Score (includes organ effects and immunotoxicity) (H, M or L): M

Magnesium hydroxide was assigned a score of Moderate for systemic/organ toxicity based on suggestive animal studies.

- No human studies were found that investigated the toxic effects of Mg(OH)₂ following inhalation exposure. Exposure of male Wistar rats to short (4.9x0.31 mm) or long (12x0.44 mm) MgSO₄/5Mg(OH)₂·3H₂O filaments inhalation, 6 hours per day, 5 days per week for up to a year was associated with a slight increase in the incidence of pulmonary lesions 1 year after cessation of exposure. A year after cessation of exposure, histopathological examination of treated animals revealed a slight increase in segmental calcification of the pulmonary artery and thickening of the lung pleura in rats exposed to either short or long filaments for 4 week or 1 year. Differences between exposed and unexposed animals were statistically significant. No significant differences in body, lung, liver, kidney, or spleen weights were detected between animals sacrificed 1 day or 1 year after a 1 year exposure to short or long filaments. No significant differences in survival were observed between animals sacrificed 1 day or 1 year after a 1 year exposure to short or long filaments (Hori 1994).
- In its review of clinical studies, the Institute of Medicine (IOM 1997) concluded that Mg²⁺ in the diet is never high enough to cause adverse effects. The IOM set a “tolerable upper intake level” (TUL) for the ingestion of magnesium (Mg²⁺) supplements of 5 mg/day for anyone over 1 year old. The TUL was based on the

approximate no-observed-adverse-effects level (NOAEL) for osmotic diarrhea in humans reported by Marken (1989), Fine (1991), Ricci (1991), and Bashir (1993). Five of the six patients reported epigastric burning or distension and two reported diarrhea.

- Decreased body weight was found to be the critical effect in B6C2F1 mice fed diets containing 0%, 0.3%, 0.6%, 1.25%, 2.5%, or 5% $\text{MgCl}_2 \cdot 6\text{H}_2\text{O}$ for 13 weeks. Intake of Mg^{2+} added to the diet was calculated to be 73, 146, 322, 650, or 1,368 mg/kg-day in treated males and 92, 190, 391, 817, and 1,660 mg/kg-day in treated females (the amount of magnesium in the basal diet was not provided). The 5% treatment group of both sexes showed a significant decrease in weight gain (15% in males and 10% in females). Males in the 2.5 and 5% group exhibited an increased incidence of renal tubular vacuolation. The authors determined that the LOAEL for this study was 650 mg/kg-day (Tanaka 1994).
- Decreased body weight and increased renal vacuolation were observed in male, but not female B6C3F1 mice fed a diet that contained 5% $\text{MgCl}_2 \cdot 6\text{H}_2\text{O}$ (Mg^{2+} at 840 mg/kg-day) for 13 weeks. No treatment-related effects were reported for male and female mice fed a diet containing 0, 0.3, 0.6, 1.25 or 2.5% $\text{MgCl}_2 \cdot 6\text{H}_2\text{O}$ for 13 weeks. The NOAEL for Mg^{2+} in this study was determined to be 587 mg/kg-day for females and 420 mg/kg-day for males (Kurata 1989).
- Decreased body weight gain (about 25% at termination of the exposure) and increases in relative brain, heart, and kidney weights compared with controls were observed in female B6C3F1 mice fed diets for 96 weeks that contained 2% $\text{MgCl}_2 \cdot 6\text{H}_2\text{O}$ (470 mg Mg^{2+} /kg-day). No treatment-related effects were observed in male mice fed diets that contained 0.5% or 2% of $\text{MgCl}_2 \cdot 6\text{H}_2\text{O}$ (68 or 336 mg/kg-day) or female mice fed diets that contained 0.5% of $\text{MgCl}_2 \cdot 6\text{H}_2\text{O}$ (87 mg/kg-day) for 96 weeks. Histopathological examination after 104 weeks of exposure revealed no treatment-related changes. Urinary, hematological, and clinical chemistry parameters and histopathological measures were not affected by treatment, except for a significant increase in serum albumin in high-dose females. Survival rates were comparable between treated and control animals. The LOAEL for this study is 470 mg/kg-d based on the treatment-related effects in high-dose female mice (Kurata 1989).

Ecotoxicity

Acute Aquatic (AA) Toxicity Score (H, M or L): L

Magnesium hydroxide was assigned a score of Low for acute aquatic toxicity based on LC_{50} values greater than 100 mg/L.

- An LC_{50} of 1,110 mg/L was estimated in fish (species not specified) (fish, 96 hour) from the measured LC_{50} s for MgCl_2 and MgSO_4 , modified by a molecular weight adjustment for $\text{Mg}(\text{OH})_2$ (Mount 1997).
- An LC_{50} of 648 mg/L was estimated in daphnia (species not identified) (daphnid, 48 hour) from the measured LC_{50} s for MgCl_2 and MgSO_4 , modified by a molecular weight adjustment for $\text{Mg}(\text{OH})_2$ (Mount 1997; Biesinger and Christensen 1972).

- An EC₅₀ of 2,111 mg/L was estimated in green algae (species not identified) (green algae, 96 hour) by using an acute to chronic ratio of 4 (U.S. EPA 2008).

Chronic Aquatic (CA) Toxicity Score (H, M or L): L

Magnesium hydroxide was assigned a score of Low for chronic aquatic toxicity based on ChV values greater than 10 mg/L.

- A ChV of 403 mg/L was estimated in fish (species not identified) (fish, time not identified) using an acute to chronic ratio of 3.3. This ratio is for daphnids and has not been validated for use with fish (U.S. EPA 2008).
- A ChV of 197 mg/L was estimated in daphnia (species not identified, length of time not identified) from the measured ChV for Mg²⁺ ion, modified by a molecular weight adjustment for Mg(OH)₂ (Suter 1996).
- A ChV of 528 mg/L was estimated in green algae (species not identified, length of time not identified) from the measured NOEC and LOEC for MgSO₄, modified by a molecular weight adjustment for Mg(OH)₂ (ECOTOX Database undated).

Environmental Fate

Persistence (P) Score (vH, H, M, or L): vH

Magnesium hydroxide was assigned a score of very High for persistence based on its inability to biodegrade in the environment.

- As a fully oxidized inorganic material, magnesium hydroxide is not expected to biodegrade, oxidize in air, or undergo hydrolysis under environmental conditions. Magnesium hydroxide does not absorb light at environmentally relevant wavelengths and is not expected to photolyze. No degradation processes for magnesium hydroxide under typical environmental conditions were identified. Chemical is identified as recalcitrant (U.S. EPA 2008).

Bioaccumulation (B) Score (vH, H, M, or L): L

Magnesium hydroxide was assigned a score of Low for bioaccumulation based on a BCF value less than 500.

- Magnesium hydroxide is not expected to be bioaccumulative based on an estimated BCF of <500 (U.S. EPA 2008).

Physical Properties

Explosivity (Ex) Hazard Rating (H, M or L): L

Magnesium hydroxide was assigned a score of Low for explosivity because no basis for concern was identified.

- Magnesium hydroxide is not explosive (IUCLID 2000).

Flammability (F) Hazard Rating (H, M or L): L

Magnesium hydroxide was assigned a score of Low for flammability because no basis for concern was identified.

- Magnesium hydroxide is not flammable (IUCLID 2000).

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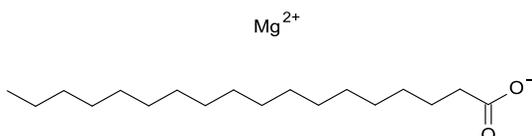


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**APPENDIX IX G: GREEN SCREEN FOR MAGNESIUM STEARATE
(CAS #557-04-0)¹⁸**

Also Called: Magnesium octadecanoate, Magnesium stearate, Magnesium stearate [JAN], Octadecanoic acid, magnesium salt, AI3-01638, Dibasic magnesium stearate, EINECS 209-150-3, HSDB 713, Magnesium distearate, Magnesium octadecanoate, Magnesium stearate, NP 1500, NS-M (salt), Octadecanoic acid, magnesium salt, Petrac MG 20NF, SM 1000, SM-P, Stearic acid, magnesium salt, Synpro 90, Synpro Magnesium Stearate 90, UNII-70097M6I30

Chemical Structure of Magnesium Stearate:



For Inorganic Chemicals:

Define Form & Physiochemical Properties

- 10. Particle size (e.g. silica of respirable size) – n/a
- 11. Structure (e.g. amorphous vs. crystalline) – Fine, white powder (HSDB 2009)
- 12. Mobility (e.g. Water solubility, volatility) – Not soluble in water (NIOSH 1994); soluble in hot alcohol (Mallinckodt Chemicals 2009).

Identify Applications/Functional Uses: Flame retardant

Green Screen Rating¹⁹: Magnesium stearate was assigned a Benchmark Score of 2 based on its High persistence (P) and Moderate irritation/corrosion (Cr) and systemic/organ toxicity (ST) (2c).

Green Screen (Version 1.0) Levels of Concern for Magnesium Stearate														
Human – Tier 1					Human – Tier 2				Eco		Fate		Physical	
C	M	R/D	ED	N	AT	Cr	Sn	ST	AA	CA	P	B	Ex	F
L	L	L	nd	nd	L	M	L	M	L	M	H	L	M	H

*Endpoints in italics were assigned using estimated values and professional judgment (Structure Activity Relationships).

¹⁸ CPA recommends independent third-party validation of all Green Screen assessments. No independent third-party validation has been done for this assessment. Companies may not make marketing claims based on a Green Screen assessment that has not undergone an independent validation.

¹⁹ For inorganic chemicals with low human and ecotoxicity across all hazard endpoints and low bioaccumulation, persistence alone will not be deemed problematic. Inorganic chemicals that are only persistent will be evaluated under the criteria for Benchmark 4.

Transformation Products and Ratings:

Identify relevant fate and transformation products (i.e., dissociation products, transformation products, valence states) and/or moieties of concern²⁰

Life Cycle Stage	Transformation Pathway	Transformation Products	CAS #	Green Screen Rating
End of Life	Dissociation	Magnesium	7439-95-4	Not present on the Red List of chemicals (CPA 2009)
End of Life	Dissociation	Octadecanoic acid	57-11-4	Not present on the Red List of chemicals (CPA 2009)
End of Life	Combustion	Carbon monoxide	630-08-0	Reproductive/developmental toxicant, neurotoxicant (CPA 2009)
End of Life	Combustion	Carbon dioxide	124-38-9	Not present on the Red List of chemicals (CPA 2009)
End of Life	Combustion	Magnesium oxide	1309-48-4	Not present on the Red List of chemicals (CPA 2009)

*The above transformation products were screened against the CPA's table of Red List chemicals (CPA 2009).

Introduction

Magnesium stearate is used as a filler material and binder in drug tablets and as an emulsification agent in cleansing products and cosmetics (HSDB 2009). Because the chemical is commonly used in pharmaceuticals, it has been listed as Generally Recognized as Safe (GRAS) by the FDA (U.S. FDA 2010).

The National Institute of Occupational Safety and Health have established a threshold limit value (TLV) for magnesium stearate of 10 mg/m³ and the Occupational Safety and Health Administration assigned a permissible exposure limit (PEL) of 15 mg/m³ (NIOSH 1994, Mallinckrodt Chemicals 2009).

Human Health – Tier 1

Carcinogenicity (C) Score (H, M or L): L

Magnesium stearate was assigned a score of Low for carcinogenicity because no basis for concern was identified.

- Not listed as a known carcinogen by IARC, NTP, U.S. EPA or CA Prop 65.
- A4- Not classifiable as a human carcinogen (HSDB 2009).

²⁰ A moiety is a discrete chemical entity that is a constituent part or component of a substance. A moiety of concern is often the parent substance itself for organic compounds. For inorganic compounds, the moiety of concern is typically a dissociated component of the substance or a transformation product.

Mutagenicity (M) and Genotoxicity Score (H, M or L): L

Magnesium stearate was assigned a score of Low for mutagenicity based on a negative Ames assay results.

- Magnesium stearate tested negative in an Ames assay (concentrations and strains not reported) both with and without metabolic activation (Litton Bionetics 1976).

Reproductive (R) and Developmental (D) Toxicity Score (H, M or L): L

Magnesium stearate was assigned a score of Low for reproductive and developmental toxicity based on negative test results in rabbits.

- Magnesium stearate did not induce developmental effects in orally treated pregnant rabbits (no other detail provided) (U.S. EPA 2009b).
- A vehicle containing 5.5% magnesium stearate did not induce any teratogenic effects at doses of 2.5 mg/kg when administered orally to pregnant rabbits (no other details provided) (Gottschewshi 1967).

Endocrine Disruption (ED) Score (H, M or L): nd

- Magnesium stearate is not listed as a potential endocrine disruptor on the EU Priority List of Suspected Endocrine Disruptors.
- Magnesium stearate is not listed as a potential endocrine disruptor on the OSPAR List of Chemicals of Possible Concern.
- Magnesium stearate is not listed as a potential endocrine disruptor on the Red List of Chemicals (CPA 2009).

Neurotoxicity (N) Score (H, M or L): nd

- Magnesium stearate is not classified as a developmental neurotoxicant (Grandjean and Landrigan 2006).
- Magnesium stearate is not listed as a potential neurotoxicant on the Red List of Chemicals (CPA 2009).

Human Health – Tier 2**Acute Mammalian (AT) Toxicity Score (H, M or L): L**

Magnesium stearate was assigned a score of Low for acute mammalian toxicity based on an oral LD₅₀ greater than 2,000 mg/kg-bw. Data is based on studies from one route of exposure in one species of animals.

- *Oral*: An LD₅₀ of >10,000 mg/kg-bw was established in the rat (U.S. EPA 2009b).

Corrosion/ Irritation (Skin/ Eye) (Cr) Score (H, M or L): M

Magnesium stearate was assigned a score of Moderate for corrosion and irritation based on conflicting results.

- *Dermal*: Magnesium stearate is a slight skin irritant (Science Lab 2008).
- *Ocular*: Magnesium stearate is slightly hazardous in the case of eye contact (Natural Sourcing 2009).

Sensitization (Sn) Score (Skin and Respiratory) (H, M or L): L

Magnesium stearate was assigned a score of Low for sensitization based on negative test results.

- Magnesium stearate does not induce dermal sensitization (no other details provided) (U.S. EPA 2009b).

Systemic/ Organ (ST) Toxicity Score (includes organ effects and immunotoxicity) (H, M or L): M

Magnesium stearate was assigned a score of Moderate for systemic/organ toxicity based on results from animal studies.

- Magnesium stearate was fed to groups of 20 male and 20 female rats (strain not reported) at levels of 0, 5, 10 and 20% in a semisynthetic diet for 3 months. Decreased weight gain was found in males in the 20% group. Urolithiasis was found in 8 males and in 7 females in the same group. Reduced relative liver weight was seen in males in the 10% and in the 20% groups, and an increased amount of iron was found in the livers of the 20% group. Nephrocalcinosis was reduced in females in the 20% group. In this experiment the no-effect-level is estimated to be 5% magnesium stearate in the diet, corresponding to 2,500 mg/kg bw/day (Sondergaard 1980).
- Magnesium stearate did not induce any adverse effects in rats when treated orally with 500 mg/kg/day for 13 months (no other details provided) (U.S. EPA 2009b).
- Magnesium stearate targets the liver and skin (Science Lab 2008).
- Repeated or prolonged exposure to magnesium stearate can produce target organs damage (Science Lab 2008).
- Grossly excessive and chronic inhalation of the dust may cause a progressive chemical pneumonitis, cyanosis, and pulmonary edema (Mallinckrodt Chemicals 2009).

Ecotoxicity**Acute Aquatic (AA) Toxicity Score (H, M or L): L**

Magnesium stearate was assigned a score of Low for acute aquatic toxicity based on professional opinion.

- ECOSAR was unable to predict E/LC₅₀ values for magnesium stearate due to its low solubility.
- Magnesium stearate is classified as a neutral organic.

Chronic Aquatic (CA) Toxicity Score (H, M or L): M

Magnesium stearate was assigned a score of Moderate for chronic aquatic toxicity based on GHS's recommendation.

- ECOSAR was unable to predict ChV values for magnesium stearate due to its low solubility.

Environmental Fate

Persistence (P) Score (vH, H, M, or L): H

Magnesium stearate was assigned a score of High for persistence based on its inability to biodegrade and a half life between 60 and 180 days in soil.

- The products of degradation are more toxic than the parent compound (Science Lab 2008).
- EPI Suite – BIOWIN model results indicate magnesium stearate is not readily biodegradable, and has a predicted degradation time of days to month. STP removal expected using BIOWIN/EPA Draft Method results indicate approximately 99% total removal, with approximately 37% due to biodegradation. Fugacity III modeling predicts approximately 84% partitioning to soil with a half-life of 75 days, and approximately 16% partitioning to water with a half-life of 38 days (U.S. EPA 2010).

Bioaccumulation (B) Score (vH, H, M, or L): L

Magnesium stearate was assigned a score of Low for bioaccumulation based on a BAF less than 500.

- BCFBAF predicts a bioaccumulation factor (BAF) of 7.079 and a log K_{ow} of 14.44 (U.S. EPA 2009a).

Physical Properties

Explosivity (Ex) Hazard Rating (H, M or L): M

Magnesium stearate was assigned a score of Moderate for explosivity based on its ability to explode when in powder form.

- Dust explosion possible if in powder or granular form and mixed with air (NIOSH 1994).

Flammability (F) Hazard Rating (H, M or L): H

Magnesium stearate was assigned a score of High for flammability based on it being combustible.

- Magnesium stearate is spontaneously combustible (HSDB 2009).
- Magnesium stearate may be combustible at high temperatures (Science Lab 2008).

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EPI Suite Results for Magnesium Stearate:

CAS Number: 557-04-0

SMILES : [Zn](OC(=O)CCCCCCCCCCCCCCCCC)OC(=O)CCCCCCCCCCCCCCCCC

CHEM : Zinc stearate

MOL FOR: C36 H70 O4 Zn1

MOL WT : 632.35

----- EPI SUMMARY (v4.00) -----

Physical Property Inputs:

Log Kow (octanol-water): -----
Boiling Point (deg C) : -----
Melting Point (deg C) : -----
Vapor Pressure (mm Hg) : -----
Water Solubility (mg/L): -----
Henry LC (atm-m3/mole) : -----

Log Octanol-Water Partition Coef (SRC):

Log Kow (KOWWIN v1.67 estimate) = 14.44

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPVP v1.43):

Boiling Pt (deg C): 675.43 (Adapted Stein & Brown method)
Melting Pt (deg C): 294.55 (Mean or Weighted MP)
VP(mm Hg,25 deg C): 2.71E-015 (Modified Grain method)
VP (Pa, 25 deg C) : 3.61E-013 (Modified Grain method)
MP (exp database): 250 deg C
Subcooled liquid VP: 7.56E-013 mm Hg (25 deg C, Mod-Grain method)
: 1.01E-010 Pa (25 deg C, Mod-Grain method)

Water Solubility Estimate from Log Kow (WSKOW v1.41):

Water Solubility at 25 deg C (mg/L): 4.609e-011
log Kow used: 14.44 (estimated)
no-melting pt equation used

Water Sol Estimate from Fragments:

Wat Sol (v1.01 est) = 6.3235e-007 mg/L

ECOSAR Class Program (ECOSAR v1.00):

Class(es) found: Neutral Organics

Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:

Bond Method : Incomplete
Group Method: Incomplete

For Henry LC Comparison Purposes:

User-Entered Henry LC: not entered
Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
HLC: 4.892E-005 atm-m3/mole (4.957E+000 Pa-m3/mole)
VP: 2.71E-015 mm Hg (source: MPBPVP)
WS: 4.61E-011 mg/L (source: WSKOWWIN)

Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1.10]:

Can Not Estimate (can not calculate HenryLC)

Probability of Rapid Biodegradation (BIOWIN v4.10):

Biowin1 (Linear Model) : 0.6634
Biowin2 (Non-Linear Model) : 0.0925

Expert Survey Biodegradation Results:

Biowin3 (Ultimate Survey Model): 2.3984 (weeks-months)

Biowin4 (Primary Survey Model): 3.4736 (days-weeks)
MITI Biodegradation Probability:
Biowin5 (MITI Linear Model) : 0.4130
Biowin6 (MITI Non-Linear Model): 0.1249
Anaerobic Biodegradation Probability:
Biowin7 (Anaerobic Linear Model): 0.8732
Ready Biodegradability Prediction: NO

Hydrocarbon Biodegradation (BioHCwin v1.01):
Structure incompatible with current estimation method!

Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
Vapor pressure (liquid/subcooled): 1.01E-010 Pa (7.56E-013 mm Hg)
Log Koa (:): not available
Kp (particle/gas partition coef. (m3/ug)):
Mackay model : 2.98E+004
Octanol/air (Koa) model: not available
Fraction sorbed to airborne particulates (phi):
Junge-Pankow model : 1
Mackay model : 1
Octanol/air (Koa) model: not available

Atmospheric Oxidation (25 deg C) [AopWin v1.92]:
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant = 42.9098 E-12 cm³/molecule-sec
Half-Life = 0.249 Days (12-hr day; 1.5E6 OH/cm³)
Half-Life = 2.991 Hrs
Ozone Reaction:
No Ozone Reaction Estimation
Fraction sorbed to airborne particulates (phi):
1 (Junge-Pankow, Mackay avg)
not available (Koa method)
Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (KOCWIN v2.00):
Koc : 8.35E+007 L/kg (MCI method)
Log Koc: 7.922 (MCI method)
Koc : 2.843E+008 L/kg (Kow method)
Log Koc: 8.454 (Kow method)

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v2.00]:
Rate constants can NOT be estimated for this structure!

Bioaccumulation Estimates (BCFBAF v3.00):
Log BCF from regression-based method = 0.500 (BCF = 3.162 L/kg wet-wt)
Log Biotransformation Half-life (HL) = 2.6112 days (HL = 408.5 days)
Log BCF Arnot-Gobas method (upper trophic) = -0.048 (BCF = 0.8945)
Log BAF Arnot-Gobas method (upper trophic) = 0.850 (BAF = 7.079)
log Kow used: 14.44 (estimated)

Volatilization from Water:
Henry LC: 4.89E-005 atm-m³/mole (calculated from VP/WS)
Half-Life from Model River: 32.66 hours (1.361 days)
Half-Life from Model Lake : 567.2 hours (23.63 days)

Removal In Wastewater Treatment:
Total removal: 94.04 percent

Total biodegradation: 0.78 percent
 Total sludge adsorption: 93.26 percent
 Total to Air: 0.00 percent
 (using 10000 hr Bio P,A,S)

Removal In Wastewater Treatment (recommended maximum 95%):

Total removal: 99.07 percent
 Total biodegradation: 37.17 percent
 Total sludge adsorption: 61.89 percent
 Total to Air: 0.00 percent
 (using Biowin/EPA draft method)

Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.177	5.98	1000
Water	15.9	900	1000
Soil	83.9	1.8e+003	1000
Sediment	0.00575	8.1e+003	0
Persistence Time: 1.21e+003 hr			

ECOSAR Results for Magnesium Stearate:

SMILES : [Mg](OC(=O)CCCCCCCCCCCCCCCCCC)OC(=O)CCCCCCCCCCCCCCCCCC

CHEM : Octadecanoic acid, magnesium salt

CAS Num: 000557-04-0

ChemID1:

ChemID2:

ChemID3:

MOL FOR: C36 H70 O4 Mg1

MOL WT : 591.26

Log Kow: 14.34 (KowWin estimate)

Melt Pt:

Wat Sol: 1.045E-010 mg/L (WskowWin estimate)

ECOSAR v1.00 Class(es) Found

 Neutral Organics

ECOSAR Class	Organism	Predicted Duration	End Pt	mg/L (ppm)
Neutral Organics	: Fish	96-hr	LC50	6.35e-009 *
Neutral Organics	: Fish	14-day	LC50	7.83e-009 *
Neutral Organics	: Daphnid	48-hr	LC50	2.22e-008 *
Neutral Organics	: Green Algae	96-hr	EC50	2.23e-006 *
Neutral Organics	: Fish	30-day	ChV	1.51e-009 *
Neutral Organics	: Daphnid		ChV	1.82e-008 *
Neutral Organics	: Green Algae		ChV	6.68e-006 *
Neutral Organics	: Fish (SW)	96-hr	LC50	3.46e-009 *
Neutral Organics	: Mysid Shrimp	96-hr	LC50	9.53e-013
Neutral Organics	: Fish (SW)		ChV	1.11e-006 *
Neutral Organics	: Mysid Shrimp (SW)		ChV	2.13e-015
Neutral Organics	: Earthworm	14-day	LC50	54.019 *

Note: * = asterisk designates: Chemical may not be soluble

enough to measure this predicted effect.

Neutral Organics:

For Fish LC50 (96-h), Daphnid LC50, Mysid: If the log Kow is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

For Fish LC50 (14-day) and Earthworm LC50: If the log Kow is greater than 6.0, or if the compound is solid and the LC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

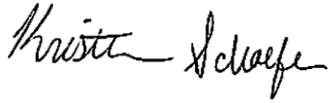
For Green Algae Acute Toxicity Values: If the log Kow of the chemical is greater than 6.4, or if the compound is solid and the EC50 exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

For All Chronic Toxicity Values: If the log Kow of the chemical is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

ECOSAR v1.00 SAR Limitations:

Maximum LogKow: 5.0 (Fish 96-hr LC50; Daphnid LC50, Mysid LC50)
Maximum LogKow: 6.0 (Fish 14-day LC50; Earthworm LC50)
Maximum LogKow: 6.4 (Green Algae EC50)
Maximum LogKow: 8.0 (ChV)
Maximum Mol Wt: 1000

Magnesium Stearate Green Screen Evaluation Prepared By:



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Associate Toxicologist
ToxServices LLC

Magnesium Stearate Green Screen Evaluation QC'd By:

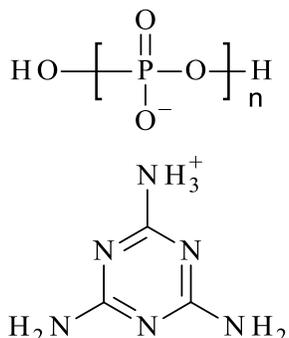


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**APPENDIX IX H: GREEN SCREEN FOR MELAMINE POLYPHOSPHATE
(CAS #218768-84-4)²¹**

Also Called: Polyphosphoric acids, compounds with melamine, Melapur 200

Chemical Structure of Melamine Polyphosphate:



***Note:** Data gaps for melamine polyphosphate (CAS #218768-84-4) were addressed using the structurally similar chemicals melamine phosphate (CAS #41583-09-9), melamine (CAS #108-78-1), and phosphate (CAS #14265-44-2) as surrogates.

For Polymers (Identify Monomers and Corresponding Properties):

% of Each Monomer – n/a

Are the monomers blocked? (Y/N) – n/a

Molecular Weight (MW) of Polymer >1,000 (U.S. EPA 2008b)

% of Polymer with – n/a

a) MW <500

b) MW <1,000

% Weight Residual Monomers – n/a

Solubility/Dispersability/Swellability – 20 g/L (U.S. EPA 2008b)

Particle Size – n/a

Overall Polymer Charge – n/a

Identify Applications/Functional Uses: Flame retardant.

Green Screen Rating²²: Melamine polyphosphate was assigned a Benchmark Score of 2 based on High systemic toxicity (ST), and Moderate carcinogenicity (C) and mutagenicity (M) (2d).

Green Screen (Version 1) Levels of Concern for Melamine Polyphosphate														
Human – Tier 1					Human – Tier 2				Eco		Fate		Physical	
C	M	R/D	ED	N	AT	Cr	Sn	ST	AA	CA	P	B	Ex	F
M	M	L	nd	nd	L	L	L	H	L	L	M	L	L	L

²¹ CPA recommends independent third-party validation of all Green Screen assessments. No independent third-party validation has been done for this assessment. Companies may not make marketing claims based on a Green Screen assessment that has not undergone an independent validation.

²² For inorganic chemicals with low human and ecotoxicity across all hazard endpoints and low bioaccumulation, persistence alone will not be deemed problematic. Inorganic chemicals that are only persistent will be evaluated under the criteria for Benchmark 4.

*Endpoints in italics were assigned using estimated values and professional judgment (Structure Activity Relationships).

Transformation Products and Ratings:

Identify relevant fate and transformation products (i.e., dissociation products, transformation products, valence states) and/or moieties of concern²³

Life Cycle Stage	Transformation Pathway	Transformation Products	CAS #	Green Screen Rating
End of Life	Combustion; Biodegradation	Melamine	108-78-1	Not present on Red List of Chemicals (CPA 2009)
End of Life	Combustion; Biodegradation	Phosphate ion	14265-44-2	Not present on Red List of Chemicals (CPA 2009)
End of Life	Combustion	Melamine pyrophosphate	15541-60-3	Not present on Red List of Chemicals (CPA 2009)
End of Life	Combustion	Phosphoric acid	7664-38-2	Not present on Red List of Chemicals (CPA 2009)
End of Life	Combustion	Hydrogen cyanide	74-90-8	Potential neurotoxicant (CPA 2009)
End of Life	Combustion	Melamine polyphosphates	20208-95-1	Not present on Red List of Chemicals (CPA 2009)

*The above transformation products were screened against the CPA's table of Red List chemicals.

Introduction

Melamine phosphates are salts of melamine and phosphoric acid. These salts have good properties of thermal stability and are commonly used as flame retardants (UNEP 1997). Melamine and its derivatives (cyanurate, phosphates) are currently used in flexible polyurethane foams, intumescent coatings, polyamides and thermoplastic polyurethanes. There were not extensive data for melamine polyphosphate. In cases of data gaps, data for melamine phosphate, and the ions for melamine and phosphate were considered.

The U.S Food and Drug Administration (U.S. FDA) established a TDI (Tolerable Daily Intake) for melamine of 0.63 mg/kg bw/day (U.S. FDA 2007). This TDI was based on the results of a 13-week rat study of melamine (see reproductive toxicity section) and incorporates safety factors totaling 100. There is recent, strong evidence to suggest that the toxicity of melamine and cyanurate is synergistic (see repeat dose toxicity section). Based on these relatively new data, the U.S. FDA applied an additional 10-fold safety

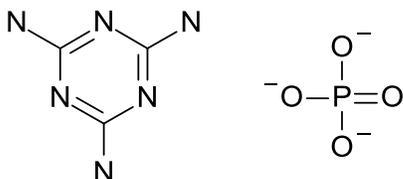
²³ A moiety is a discrete chemical entity that is a constituent part or component of a substance. A moiety of concern is often the parent substance itself for organic compounds. For inorganic compounds, the moiety of concern is typically a dissociated component of the substance or a transformation product.

factor to yield a combined safety factor of 1000-fold. Therefore, a TDI of 0.063 mg/kg bw/day was proposed (U.S. FDA 2008).

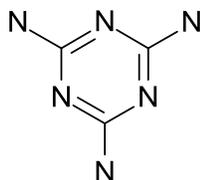
Melamine is degraded by three successive deamination reactions to ammeline (4,6-diamino-2-hydroxy-1,3,5-triazine), ammelide (6-amino-2,4-dihydroxy-1,3,5-triazine) and cyanuric acid(s-triazine-2,4,6-triol).

Melamine and phosphate are the expected breakdown products of melamine phosphate in the environment. The following chemical screen primarily uses toxicity data on melamine when the database for melamine phosphate is absent. Phosphate ion is also evaluated with regard to environmental parameters, but is not included in the human health analysis, as it is not expected to pose a risk to humans (U.S. EPA 1993).

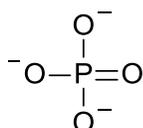
Chemical Structure of Surrogate:



Melamine phosphate (CAS #41583-09-9)



Melamine (CAS #108-78-1)



Phosphate (CAS #14265-44-2)

Human Health – Tier 1

Carcinogenicity (C) Score (H, M or L): M

Because no relevant carcinogenicity data for melamine polyphosphate were identified, the structurally similar melamine was used as a surrogate. Melamine polyphosphate was assigned a score of Moderate for carcinogenicity due to the conflicting evidence of carcinogenic properties for the surrogate, melamine, which induced bladder carcinomas in several animal studies.

***Note:** Unless specifically noted, information regarding animal strain or sex, dose, route of exposure, duration of experiment, or if these studies followed GLP guidelines was not provided by the authors of these studies.

Melamine polyphosphate

- Melamine polyphosphate is not listed as a known carcinogen by IARC, NTP, U.S. EPA, or CA Prop 65.

Melamine

- Significant formation of transitional cell carcinomas in the urinary bladder of male rats and significant chronic inflammation in the kidney of dosed female rats were observed. Carcinoma formation was significantly correlated with the incidence of bladder stones. A transitional-cell papilloma was observed in the urinary bladder of a single high dose male rat, and compound related lesions were observed in the urinary tract of dosed animals. Based on the mechanical nature of tumor formation, FDA and EPA considered melamine noncarcinogenic (U.S. EPA 2008).
- Increased incidence of acute and chronic inflammation and epithelial hyperplasia of the urinary bladder was observed in male mice. Bladder stones and compound related lesions were observed in the urinary tract of test animals. Melamine was not considered carcinogenic. No information concerning dose, route of administration, or other study details were provided (U.S. EPA 2008).
- Melamine-induced proliferative lesions of the rat urinary tract were directly due to the irritative stimulation of calculi, and not to molecular interactions between melamine or its metabolites with the bladder epithelium (U.S. EPA 2008).
- Water intake, used as an index of urinary output, was increased by NaCl treatment. Calculus formation resulting from melamine administration was suppressed dose-dependently by the simultaneous NaCl treatment. The main constituents of calculi were melamine and uric acid (total contents 61.1–81.2%). The results indicate that melamine-induced proliferative lesions of the urinary tract of rats were directly due to the irritative stimulation of calculi, and not molecular interactions between melamine itself or its metabolites with the bladder epithelium (U.S. EPA 2008).
- As an initiator, melamine caused no significant increase in papillomas per mouse when compared to controls (U.S. EPA 2008).
- Diffuse papillary hyperplasia of the bladder epithelium and bladder calculi were observed in all melamine treated rats. Elevated spermidine/spermine N1-acetyltransferase (SAT) activity following melamine treatment was considered to be an indicator of cell proliferation (U.S. EPA 2008).
- Bladder tumors were only observed in the male rat and not in female rats or mice of either sex. An experiment did not reveal melamine as a tumor initiator. The formation of bladder stones and subsequent irritation of the bladder epithelium are necessary for tumor induction. Melamine is only indirectly responsible for the occurrence of bladder tumors. The incidence of calculi is dose dependent. The mechanism for tumor production is a non-genotoxic one. A threshold of 126 mg/kg for the formation of neoplasms can therefore be established. This value is based on a 2-year NTP feeding study with male Fisher 344 rats. The toxicity potential of melamine itself is considered low by the Consumer Product Safety Commission (Thomas and Brundage 2004).

Mutagenicity (M) and Genotoxicity Score (H, M or L): M

Because no relevant mutagenicity or genotoxicity data for melamine polyphosphate were identified, the structurally similar melamine was used as a surrogate. Melamine polyphosphate was assigned a score of Moderate for mutagenicity and genotoxicity due to the conflicting evidence of genotoxic properties for the surrogate, melamine, which induced chromosomal damage in several animal studies.

***Note:** Unless specifically noted, information regarding animal strain or sex, dose, route of exposure, duration of experiment, or if these studies followed GLP guidelines was not provided by the authors of these studies.

Melamine

- Bacterial forward mutation assay: Negative with and without liver activation (U.S. EPA 2008).
- *In vitro* mouse lymphoma test: Negative with and without liver activation (U.S. EPA 2008).
- *In vivo* mouse micronucleus test: The initial test gave a positive trend (P=0.003) for chromosomal damage; however, both peripheral blood smears and the repeat bone marrow test were negative. The overall conclusion was that melamine does not induce chromosomal damage (U.S. EPA 2008).
- *In vitro* chromosomal aberrations test: Negative in Chinese hamster ovary cells (CHO) with and without liver activation (U.S. EPA 2008).
- *In vitro* sister chromatid exchange assay: Negative in Chinese hamster ovary cells (CHO) with and without liver activation (U.S. EPA 2008).
- *In vivo* chromosome aberrations test in mice: Positive (U.S. EPA 2008).
- *In vivo* sister chromatid exchange assay in mice: Positive (U.S. EPA 2008)
- SOS/*umu* test: Negative for its ability to result in DNA damage and induce the expression of the *umu* operon (U.S. EPA 2008)
- Sex-linked recessive lethal/reciprocal translocation: Results were considered equivocal based on 0.18% and 0.36% total lethals following oral and injection exposure, respectively, compared to control total lethals of 0.07% for oral and 0.09% for injection (U.S. EPA 2008).
- *In vitro* flow cytometric (FCM) DNA repair assay: Negative for genotoxic effects (U.S. EPA 2008).
- Microscreen assay: Positive for genetic toxicity in *E. coli* WP2 *uvrA* assay (U.S. EPA 2008).

Reproductive (R) and Developmental (D) Toxicity Score (H, M or L): L

Because no relevant reproductive or developmental toxicity data were identified for melamine polyphosphate, the structurally similar melamine was used as a surrogate. Melamine polyphosphate was assigned a score of Low for reproductive and developmental toxicity because no basis of concern was identified.

***Note:** Unless specifically noted, information regarding animal strain or sex, dose, route of exposure, duration of experiment, or if these studies followed GLP guidelines was not provided by the authors of these studies.

Melamine

- Reproductive dysfunction was observed at 0.5 mg/m³ and included effects on spermatogenesis (genetic material, sperm morphology, motility, and count), effects on the embryo/fetus (fetal death), preimplantation mortality (reduction in the number of implants per female), and total number of implants per corpora lutea (U.S EPA 2008).
- Mammary glands, ovaries, prostate, seminal vesicles, testes and uterus were examined macroscopically and microscopically in 13-week and in chronic toxicity studies with rats and mice and were found to be unaffected by melamine at each of the doses used. The lowest NOEL for systemic toxicity in these studies was 63 mg/kg/day (UNEP 1998).
- Melamine was not teratogenic in an investigation with rats. The NOEL for the fetuses was 1060 mg/kg/day, the highest dose tested. A maternal NOEL of 400 mg/kg/day was established based on decreased body weight and feed consumption and hematuria (UNEP 1998).

Endocrine Disruption (ED) Score (H, M or L): nd

- Melamine polyphosphate is not listed as a potential endocrine disruptor on the EU Priority List of Suspected Endocrine Disruptors.
- Melamine polyphosphate is not listed as a potential endocrine disruptor on the OSPAR List of Chemicals of Possible Concern.
- Melamine polyphosphate is not listed as a potential endocrine disruptor on the Red List of Chemicals (CPA 2009).

Neurotoxicity (N) Score (H, M or L): nd

- Melamine polyphosphate is not classified as a developmental neurotoxicant (Grandjean and Landrigan 2006).
- Melamine polyphosphate is not listed as a potential neurotoxicant on the Red List of Chemicals (CPA 2009).

Human Health – Tier 2

Acute Mammalian (AT) Toxicity Score (H, M or L): L

Melamine polyphosphate was assigned a score of Low for acute mammalian toxicity based on oral and dermal LD₅₀ values of 2,000 or less mg/kg-bw from analog data. Data is from three different chemicals using two different routes of exposure in three different species of animals.

Melamine polyphosphate

- *Oral*: An LD₅₀ of > 2,000 mg/kg was determined in the rat (U.S. EPA 2008).

Melamine phosphate

- *Oral*: An LD₅₀ of > 2,000 mg/kg was determined in the mouse (Ciba 2005).
- *Dermal*: An LD₅₀ of > 2,000 mg/kg was determined in the rabbit (Hummel Croton 2009).

Melamine

- *Oral*: An LD₅₀ of 3,161 mg/kg (male) and 3,828 mg/kg (female) was determined in the rat (U.S. EPA 2008).
- *Oral*: An LD₅₀ of > 6,400 mg/kg-bw was determined in the rat (U.S. EPA 2008).
- *Oral*: An LD₅₀ of 3,296 mg/kg (male) and 7,014 mg/kg (female) was determined in the mouse (U.S. EPA 2008).
- *Oral*: An LD₅₀ of 4,550 mg/kg was determined in the mouse (U.S. EPA 2008).
- *Dermal*: An LD₅₀ of > 1,000 mg/kg was determined in the rabbit (U.S. EPA 2008).

Corrosion/ Irritation (Skin/ Eye) (Cr) Score (H, M or L): L

Melamine polyphosphate was assigned a score of Low for corrosion and irritation because no cause for concern was identified.

Melamine polyphosphate

- *Dermal*: Melamine polyphosphate was not irritating (no other data provided) (U.S. EPA 2008).
- *Ocular*: Melamine polyphosphate was slightly irritating (no other data provided) (U.S. EPA 2008).

Sensitization (Sn) Score (Skin and Respiratory) (H, M or L): L

Because no relevant sensitization data for melamine polyphosphate were identified, the structurally similar melamine phosphate and melamine were used as surrogates. Melamine polyphosphate was assigned a score of Low for sensitization because no basis for concern was identified.

Melamine Phosphate

- Melamine phosphate was not sensitizing in guinea pigs under Test Method OECD 406 (Ciba 2005).

Melamine

- Melamine was not sensitizing in human or guinea pig repeat insult patch test (UNEP 1998).

Systemic/ Organ (ST) Toxicity Score (includes organ effects and immunotoxicity) (H, M or L): H

Because no relevant systemic/organ toxicity data for melamine polyphosphate were identified, the structurally similar melamine was used as a surrogate. Melamine polyphosphate was assigned a score of High for systemic/organ toxicity based on analog data suggesting melamine causes kidney and bladder toxicity in animals.

***Note:** Unless specifically noted, information regarding animal strain or sex, dose, route of exposure, duration of experiment, or if these studies followed GLP guidelines was not provided by the authors of these studies.

Melamine

- Clinical signs observed during a 28-day repeat-dose study in rats included a dose-related increase in pilo-erection, lethargy, bloody urine spots in the cage and on the pelage of animals, and chromodacryorrhea. The incidence of urinary bladder calculi and urinary bladder hyperplasia in treated animals was dose dependant, with a significant relationship between the calculi and hyperplasia. Calculi composition indicated the presence of an organic matrix containing melamine,

- phosphorus, sulfur, potassium, and chloride. Crystals of dimelamine monophosphate were identified in the urine. The NOAEL was estimated to be 2000 ppm (240 mg/kg/day), excluding the observed increase in water consumption and the incidence of crystalluria. The LOAEL was determined to be 4,000 ppm (475 mg/kg/day) based on the formation of calculus (U.S. EPA 2008).
- Following a 90-day repeat-dose study in rats, one male rat receiving 18000 ppm and two males receiving 6,000 ppm died. Mean body weight gain and feed consumption were reduced. Stones and diffuse epithelial hyperplasia in the urinary bladders were observed. Focal epithelial hyperplasia was observed in only 1 male. A second and third 13-week repeated dose toxicity study was conducted in rats at a dose range of 750 to 18000 ppm in order to determine the No Observed Adverse Effect Level; however, bladder stones were observed at all dose levels. At 18000 ppm, stones occurred in diets with and without the addition of ammonium chloride (U.S. EPA 2008).
 - A single female mouse died after receiving 9000 ppm in a 90-day repeat-dose study. Mean body weight gain relative to controls was depressed. The incidence of mice with bladder stones was dose-related and was greater in males than in females. Sixty percent of mice having bladder ulcers also had urinary bladder stones. Bladder ulcers were multifocal or associated with inflammation (cystitis). Epithelial hyperplasia and bladder stones were observed together in 2 mice. Also, epithelial cell atypia was seen. No observed adverse effects were noted at 6000 ppm (U.S. EPA 2008).
 - Following the incidence of melamine contamination in pet food, a pilot study was carried out in which cats (one per dose) were fed melamine, cyanuric acid, or a combination of both. For the melamine only group, one cat was fed 0.5% (181 mg/kg/day) and one cat, 1% (44-121 mg/kg/day) of the chemical for 11 days. In the cyanuric acid only group, one cat was fed 0.2% (49 mg/kg/day) for 4 days, 0.5% (121 mg/kg/day) for 3 days, and then 1% (243 mg/kg/day) for 3 days. In the final group, one cat received 32 mg/kg of each compound, one cat received 121 mg/kg of each compound, and one cat received 181 mg/kg of each compound for one day. On the second day, cats ate nothing or very little. The estimated doses were 2 mg/kg, 10 mg/kg, or 54 mg/kg of each compound. Cats dosed with a combination experienced acute renal failure and had to be euthanized after 48 hours. Findings included amorphous, rounded and fan-shaped crystals in the urine, and histologic lesions in the kidneys, the severity of which corresponded to the dose²⁴. No effect on any renal parameter was observed in cats fed melamine or cyanuric acid alone (Puschner 2007).
 - 400 mg/kg of either melamine or cyanuric acid or melamine and cyanuric acid was fed daily for 3 days to 75 fish, 4 pigs, and 1 cat. Animals were euthanized 1, 3, 6, 10, or 14 days later. All animals fed the combination of melamine and cyanuric acid developed renal crystals arranged in radial spheres. Melamine and cyanuric acid residues were identified in edible tissues of fish (Reimschuessel 2008).

Ecotoxicity

²⁴ The GHS category for toxic effects produced from a single exposure at ≤ 300 mg/kg/day or from multiple exposures at ≤ 2000 mg/kg/day is category 1.

Acute Aquatic (AA) Toxicity Score (H, M or L): L

Because no relevant acute aquatic toxicity data were identified for melamine polyphosphate and EPI Suite did not produce any results for ecotoxicity data, the structurally similar melamine phosphate, melamine, and phosphate were used as surrogates. Melamine polyphosphate was assigned a score of Low for acute aquatic toxicity based on L/EC₅₀ values of 100 mg/L or greater.

Melamine Phosphate

- An LC₅₀ of 100 mg/L was identified in a freshwater fish species (96 hour) (Ciba 2005).
- An EC₅₀ of > 100 mg/L was identified *Daphnia magna* (aquatic invertebrate, 48 hour) (Ciba 2005).

Melamine

- An LC₅₀ of > 500 mg/L was identified in *Leuciscus idus melanotus* (freshwater fish, 96 hour) (U.S. EPA 2008).
- An LC₅₀ of > 3,000 mg/L was identified in *Poecilia reticulata* (freshwater fish, 96 hour) (UNEP 1998).
- An LC₅₀ of > 2,000 mg/L was identified in *Daphnia magna* (aquatic invertebrate, 48 hour) (U.S. EPA 2008).
- An EC₅₀ of > 2,000 mg/L was identified in *Daphnia magna* (aquatic invertebrate, 48 hour) (UNEP 1998).
- An EC₅₀ of 940 mg/L was identified in *Scenedesmus pannonicus* (green algae, 96 hour) (U.S. EPA 2008).

Phosphate

- This chemical is designated to the ECOSAR class neutral organics. The most conservative estimated L/EC₅₀ acute values for fish (96-hr), daphnid (48-hr), and green algae (96-hr) are >100 mg/L (U.S. EPA 2009).

Chronic Aquatic (CA) Toxicity Score (H, M or L): L

Because no chronic aquatic toxicity data were identified for melamine polyphosphate and EPI Suite did not produce any results for ecotoxicity data, the structurally similar melamine and phosphate were used as surrogates. Melamine polyphosphate was assigned a score of Low for chronic aquatic toxicity based on NOEC values greater than 10 mg/L.

Melamine

- An NOEC of 1,000 mg/L was identified in *Jordanella floridae* (freshwater fish, 35 day) (U.S. EPA 2008).
- An NOEC of < 125 to > 1,000 mg/L was identified in a freshwater fish species (UNEP 1998).
- An LC₅₀ of 32-56 mg/L was identified in *Daphnia magna* (aquatic invertebrate, 21 day) (U.S. EPA 2008).
- An LC₅₀ of > 32 mg/L was identified in *Daphnia magna* (aquatic invertebrate, 21 day) (UNEP 1998).
- An NOEC of 18 mg/L was identified in *Daphnia magna* (aquatic invertebrate, 21 day) (UNEP 1998).

- An EC₅₀ of 1,680 mg/L was identified in an aquatic plant species (14 day) (UNEP 1998).

Phosphate

- This chemical is designated to the ECOSAR class neutral organics. The most conservative estimated L/EC₅₀ chronic values for fish (30-day), daphnid (duration not given), and green algae (duration not given) are >100 mg/L (U.S. EPA 2009).

Environmental Fate

Persistence (P) Score (vH, H, M, or L): M

Because no relevant persistence data for melamine polyphosphate were identified, the structurally similar melamine phosphate, melamine, and phosphate were used as surrogates. Melamine polyphosphate was assigned as score of Moderate for persistence based on analog data suggesting melamine polyphosphate will not biodegrade rapidly.

Melamine polyphosphate

- Based on evidence from melamine, melamine polyphosphate is expected to show moderate persistence and will not biodegrade rapidly (U.S. EPA 2008)

Melamine phosphate

- EPI Suite was unable to predict the environmental fate of melamine phosphate. Because it is a salt, it is expected to dissociate readily in the environment. Therefore, it is appropriate to evaluate the persistence of the two component ions instead.
- Above ~200°C melamine phosphate will react to melamine pyro-phosphate with release of reaction water, which will result in a heat sink. Above ~260°C melamine-pyrophosphate will react under release of reaction water to melamine-polyphosphates which again results in a heat sink effect. Above 350°C, melamine-polyphosphate undergoes endothermic decomposition and releases phosphoric acid (Ciba 2005).

Melamine

- A standard 5-day biochemical oxygen demand (BOD) test indicated melamine was not biodegradable (Saski 1970).
- Pure culture studies of *Pseudomonas* strain A exposed to 3mM melamine indicated that melamine is degraded to ammeline and eventually cyanuric acid (Jutzi 1982).
- Water is the most relevant compartment in the environmental fate of the substance (UNEP 1998).
- In water, melamine is expected to adsorb to sediment at acidic pHs (Weber 1970).
- Melamine is not expected to undergo hydrolysis in the environment due to the lack of functional groups that hydrolyze under environmental conditions (Lyman 1990).
- Melamine can be hydrolyzed by mineral acid or inorganic alkali (Crews 2005).

Phosphate

- The phosphate anion is expected to adsorb strongly to soil or colloidal particles in the water column. Salts of phosphoric acid generally dissociate (U.S EPA 1993).

Bioaccumulation (B) Score (vH, H, M, or L): L

Melamine polyphosphate was assigned a score of Low for bioaccumulation based on professional opinion and analog data that suggests the chemical will not bioaccumulate.

Melamine polyphosphate

- Because of its high water solubility (20g/L), the bioconcentration factor (BCF) is expected to be <1,000 (U.S. EPA 2008).

Melamine

- The bioaccumulation potential of melamine is low. No remarkable contribution of food from aquatic organisms to the uptake of melamine in humans is therefore expected (UNEP 1998).

Phosphate

- BCFBAF predicts a bioconcentration factor (BCF) of 3.16 for phosphate (U.S. EPA 2010)

Physical Properties**Explosivity (Ex) Hazard Rating (H, M or L): L**

Melamine polyphosphate was assigned a score of Low for reactivity because no basis for concern was identified.

- Melamine polyphosphate is not explosive (U.S. EPA 2008).

Flammability (F) Hazard Rating (H, M or L): L

Melamine polyphosphate was assigned a score of Low for flammability because no basis for concern was identified.

- Melamine polyphosphate is not flammable (U.S. EPA 2008).

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EPI Suite Results for Melamine:

CAS Number: 108-78-1
SMILES : n(c(nc(n1)N)N)c1N
CHEM : 1,3,5-Triazine-2,4,6-triamine
MOL FOR: C3 H6 N6
MOL WT : 126.12

----- EPI SUMMARY (v4.00) -----

Physical Property Inputs:

Log Kow (octanol-water): -----
Boiling Point (deg C) : -----
Melting Point (deg C) : -----
Vapor Pressure (mm Hg) : -----
Water Solubility (mg/L): -----
Henry LC (atm-m³/mole) : -----

Log Octanol-Water Partition Coef (SRC):

Log Kow (KOWWIN v1.67 estimate) = -0.38
Log Kow (Exper. database match) = -1.37
Exper. Ref: HANSCH,C ET AL. (1995)

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPVP v1.43):

Boiling Pt (deg C): 329.78 (Adapted Stein & Brown method)
Melting Pt (deg C): 133.08 (Mean or Weighted MP)
VP(mm Hg,25 deg C): 8.93E-008 (Modified Grain method)
VP (Pa, 25 deg C) : 1.19E-005 (Modified Grain method)
MP (exp database): 345 dec deg C
VP (exp database): 3.59E-10 mm Hg (4.79E-008 Pa) at 20 deg C
Subcooled liquid VP: 5.25E-007 mm Hg (20 deg C, exp database VP)
: 7E-005 Pa (20 deg C, exp database VP)

Water Solubility Estimate from Log Kow (WSKOW v1.41):

Water Solubility at 25 deg C (mg/L): 1e+006
log Kow used: -1.37 (expkow database)
no-melting pt equation used
Water Sol (Exper. database match) = 3230 mg/L (20 deg C)
Exper. Ref: YALKOWSKY,SH & HE,Y (2003)

Water Sol Estimate from Fragments:

Wat Sol (v1.01 est) = 1040.5 mg/L

ECOSAR Class Program (ECOSAR v1.00):

Class(es) found:
Anilines (amino-meta)
Triazines
Melamines

Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:

Bond Method : 1.89E-013 atm-m³/mole (1.92E-008 Pa-m³/mole)
Group Method: Incomplete
Exper Database: 1.84E-14 atm-m³/mole (1.86E-009 Pa-m³/mole)

For Henry LC Comparison Purposes:

User-Entered Henry LC: not entered
Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
HLC: 1.482E-014 atm-m³/mole (1.502E-009 Pa-m³/mole)
VP: 8.93E-008 mm Hg (source: MPBPVP)

WS: 1E+006 mg/L (source: WSKOWWIN)

Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1.10]:

Log Kow used: -1.37 (exp database)

Log Kaw used: -12.124 (exp database)

Log Koa (KOAWIN v1.10 estimate): 10.754

Log Koa (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10):

Biowin1 (Linear Model) : -0.0042

Biowin2 (Non-Linear Model) : 0.0000

Expert Survey Biodegradation Results:

Biowin3 (Ultimate Survey Model): 2.2697 (weeks-months)

Biowin4 (Primary Survey Model): 3.2831 (days-weeks)

MITI Biodegradation Probability:

Biowin5 (MITI Linear Model) : -0.0193

Biowin6 (MITI Non-Linear Model): 0.0000

Anaerobic Biodegradation Probability:

Biowin7 (Anaerobic Linear Model): -0.0756

Ready Biodegradability Prediction: NO

Hydrocarbon Biodegradation (BioHCwin v1.01):

Structure incompatible with current estimation method!

Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:

Vapor pressure (liquid/subcooled): 7E-005 Pa (5.25E-007 mm Hg)

Log Koa (Koawin est): 10.754

Kp (particle/gas partition coef. (m3/ug)):

Mackay model : 0.0429

Octanol/air (Koa) model: 0.0139

Fraction sorbed to airborne particulates (phi):

Junge-Pankow model : 0.608

Mackay model : 0.774

Octanol/air (Koa) model: 0.527

Atmospheric Oxidation (25 deg C) [AopWin v1.92]:

Hydroxyl Radicals Reaction:

OVERALL OH Rate Constant = 0.6596 E-12 cm³/molecule-sec

Half-Life = 16.216 Days (12-hr day; 1.5E6 OH/cm³)

Ozone Reaction:

No Ozone Reaction Estimation

Fraction sorbed to airborne particulates (phi):

0.691 (Junge-Pankow, Mackay avg)

0.527 (Koa method)

Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (KOCWIN v2.00):

Koc : 32.28 L/kg (MCI method)

Log Koc: 1.509 (MCI method)

Koc : 1 L/kg (Kow method)

Log Koc: 0.000 (Kow method)

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v2.00]:

Rate constants can NOT be estimated for this structure!

Bioaccumulation Estimates (BCFBAF v3.00):

Log BCF from regression-based method = 0.500 (BCF = 3.162 L/kg wet-wt)

Log Biotransformation Half-life (HL) = -3.1607 days (HL = 0.0006907 days)
 Log BCF Arnot-Gobas method (upper trophic) = -0.049 (BCF = 0.8938)
 Log BAF Arnot-Gobas method (upper trophic) = -0.049 (BAF = 0.8938)
 log Kow used: -1.37 (expkow database)

Volatilization from Water:

Henry LC: 1.84E-014 atm-m³/mole (Henry experimental database)
 Half-Life from Model River: 3.573E+010 hours (1.489E+009 days)
 Half-Life from Model Lake : 3.898E+011 hours (1.624E+010 days)

Removal In Wastewater Treatment:

Total removal: 1.85 percent
 Total biodegradation: 0.09 percent
 Total sludge adsorption: 1.75 percent
 Total to Air: 0.00 percent
 (using 10000 hr Bio P,A,S)

Removal In Wastewater Treatment:

Total removal: 21.97 percent
 Total biodegradation: 20.53 percent
 Total sludge adsorption: 1.44 percent
 Total to Air: 0.00 percent
 (using Biowin/EPA draft method)

Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	3.41e-007	389	1000
Water	25	900	1000
Soil	74.9	1.8e+003	1000
Sediment	0.086	8.1e+003	0

Persistence Time: 1.37e+003 hr

ECOSAR Results for Melamine:

SMILES : n(c(nc(n1)N)N)c1N
 CHEM : 1,3,5-Triazine-2,4,6-triamine
 CAS Num: 000108-78-1
 ChemID1:
 ChemID2:
 ChemID3:
 MOL FOR: C3 H6 N6
 MOL WT : 126.12
 Log Kow: -0.38 (KowWin estimate)
 Melt Pt:
 Wat Sol: 3230 mg/L (experimental database)

ECOSAR v1.00 Class(es) Found

 Anilines (amino-meta)
 Triazines
 Melamines

ECOSAR Class	Organism	Predicted		
		Duration	End Pt	mg/L (ppm)
Anilines (amino-meta)	: Fish	96-hr	LC50	1863.183

Anilines (amino-meta)	: Daphnid	48-hr	LC50	6.837
Anilines (amino-meta)	: Green Algae	96-hr	EC50	2.789
Anilines (amino-meta)	: Fish		ChV	186.204 !
Anilines (amino-meta)	: Daphnid		ChV	0.069
Anilines (amino-meta)	: Green Algae		ChV	0.054 !

Triazines	: Fish	96-hr	LC50	42792.074 *
Triazines	: Daphnid	48-hr	LC50	4418.740 *
Triazines	: Green Algae	96-hr	EC50	276.519
Triazines	: Fish		ChV	1007.473 !
Triazines	: Daphnid	21-day	ChV	150.580
Triazines	: Green Algae		ChV	39.539

Melamines	: Fish	96-hr	LC50	390.882
Melamines	: Daphnid	48-hr	LC50	274.094
Melamines	: Green Algae	96-hr	EC50	324.968
Melamines	: Fish		ChV	1102.529
Melamines	: Daphnid		ChV	16.591 !
Melamines	: Green Algae		ChV	81.248 !

=====

Neutral Organic SAR	: Fish	96-hr	LC50	10068.581 *
(Baseline Toxicity)	: Daphnid	48-hr	LC50	4356.359 *
	: Green Algae	96-hr	EC50	706.784
	: Fish		ChV	1007.473
	: Daphnid		ChV	264.059
	: Green Algae		ChV	165.581

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect.

Note: ! = exclamation designates: The toxicity value was determined from a predicted SAR using established acute-to-chronic ratios and ECOSAR regression techniques which are documented in the supporting Technical Reference Manual. When possible, this toxicity value should be considered in a weight of evidence approach.

Anilines (amino-meta):

For Fish and Daphnid Acute Toxicity Values: If the log Kow of the chemical is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

For Green Algae Acute Toxicity Values: If the log Kow of the chemical is greater than 6.4, or if the compound is solid and the EC50 exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

For All Chronic Toxicity Values: If the log Kow of the chemical is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

ECOSAR v1.00 SAR Limitations:

Maximum LogKow: 5.0 (LC50)
 Maximum LogKow: 6.4 (EC50)
 Maximum LogKow: 8.0 (ChV)
 Maximum Mol Wt: 1000

Triazines:

For Fish and Daphnid Acute Toxicity Values: If the log Kow of the chemical is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

For Green Algae Acute Toxicity Values: If the log Kow of the chemical is greater than 6.4, or if the compound is solid and the EC50 exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

For All Chronic Toxicity Values: If the log Kow of the chemical is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

ECOSAR v1.00 SAR Limitations:

Maximum LogKow: 5.0 (LC50)
Maximum LogKow: 6.4 (EC50)
Maximum LogKow: 8.0 (ChV)
Maximum Mol Wt: 1000

Melamines :

For Fish and Daphnid Acute Toxicity Values: If the log Kow of the chemical is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

For Green Algae Acute Toxicity Values: If the log Kow of the chemical is greater than 6.4, or if the compound is solid and the EC50 exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

For All Chronic Toxicity Values: If the log Kow of the chemical is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

ECOSAR v1.00 SAR Limitations:

Maximum LogKow: 5.0 (LC50)
Maximum LogKow: 6.4 (EC50)
Maximum LogKow: 8.0 (ChV)
Maximum Mol Wt: 1000

Baseline Toxicity SAR Limitations:

Maximum LogKow: 5.0 (Fish 96-hr LC50; Daphnid LC50)
Maximum LogKow: 6.4 (Green Algae EC50)
Maximum LogKow: 8.0 (ChV)
Maximum Mol Wt: 1000

EPI Suite Results for Phosphate:

CAS Number: 14265-44-2
SMILES : OP(=O)(O)O
CHEM : PHOSPHATE
MOL FOR: H3 O4 P1

MOL WT : 98.00

----- EPI SUMMARY (v4.00) -----

Physical Property Inputs:

Log Kow (octanol-water): -----
Boiling Point (deg C) : -----
Melting Point (deg C) : -----
Vapor Pressure (mm Hg) : -----
Water Solubility (mg/L): -----
Henry LC (atm-m³/mole) : -----

Log Octanol-Water Partition Coef (SRC):

*** WARNING: Inorganic Compound (Outside Estimation Domain)
Log Kow (KOWWIN v1.67 estimate) = -0.77

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPVP v1.43):

*** WARNING: Inorganic Compound (Outside Estimate Domain) ***
*** WARNING: Estimations NOT VALID ***
Boiling Pt (deg C): 480.00 (Adapted Stein & Brown method)
Melting Pt (deg C): 90.27 (Mean or Weighted MP)
VP(mm Hg,25 deg C): 6.09E-011 (Modified Grain method)
VP (Pa, 25 deg C) : 8.12E-009 (Modified Grain method)
MP (exp database): 42.35 deg C
Subcooled liquid VP: 8.76E-011 mm Hg (25 deg C, Mod-Grain method)
: 1.17E-008 Pa (25 deg C, Mod-Grain method)

Water Solubility Estimate from Log Kow (WSKOW v1.41):

*** WARNING: Inorganic Compound (Outside Estimation Domain)**
Water Solubility at 25 deg C (mg/L): 5.386e+005
log Kow used: -0.77 (estimated) no-melting pt equation used

Water Sol Estimate from Fragments:

*** WARNING: Inorganic Compound (Outside Estimation Domain)***
*** WARNING: Wat Sol Estimation NOT Valid ***
Wat Sol (v1.01 est) = 1e+006 mg/L

ECOSAR Class Program (ECOSAR v1.00):

Class(es) found:
Neutral Organics

Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:

*** WARNING: Inorganic Compound (Outside Estimation Domain) **
*** WARNING: Estimation NOT VALID **
Bond Method : 7.60E-015 atm-m³/mole (7.70E-010 Pa-m³/mole)
Group Method: Incomplete

For Henry LC Comparison Purposes:

User-Entered Henry LC: not entered
Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
HLC: 1.458E-017 atm-m³/mole (1.477E-012 Pa-m³/mole)
VP: 6.09E-011 mm Hg (source: MPBPVP)
WS: 5.39E+005 mg/L (source: WSKOWWIN)

Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1.10]:

*** WARNING: Inorganic Compound (Outside Estimation Domain)**
*** WARNING: Estimation NOT VALID ***
Log Kow used: -0.77 (KowWin est)
Log Kaw used: -12.508 (HenryWin est)
Log Koa (KOAWIN v1.10 estimate): 11.738

Log Koa (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10):

*** WARNING: Inorganic Compound (Outside Estimation Domain)**

*** WARNING: Estimation NOT VALID ***

Biowin1 (Linear Model) : 0.7009

Biowin2 (Non-Linear Model) : 0.8344

Expert Survey Biodegradation Results:

Biowin3 (Ultimate Survey Model): 2.9826 (weeks)

Biowin4 (Primary Survey Model) : 3.7064 (days-weeks)

MITI Biodegradation Probability:

Biowin5 (MITI Linear Model) : 0.4206

Biowin6 (MITI Non-Linear Model): 0.4247

Anaerobic Biodegradation Probability:

Biowin7 (Anaerobic Linear Model): 0.8361

Ready Biodegradability Prediction: NO

Hydrocarbon Biodegradation (BioHCwin v1.01):

Structure incompatible with current estimation method!

Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:

Vapor pressure (liquid/subcooled): 1.17E-008 Pa (8.76E-011 mm Hg)

Log Koa (Koawin est) : 11.738

Kp (particle/gas partition coef. (m³/ug)):

Mackay model : 257

Octanol/air (Koa) model: 0.134

Fraction sorbed to airborne particulates (phi):

Junge-Pankow model : 1

Mackay model : 1

Octanol/air (Koa) model: 0.915

Atmospheric Oxidation (25 deg C) [AopWin v1.92]:

*** WARNING: Inorganic Compound (Outside Estimation Domain)**

Hydroxyl Radicals Reaction:

OVERALL OH Rate Constant = 0.4200 E-12 cm³/molecule-sec

Half-Life = 25.467 Days (12-hr day; 1.5E6 OH/cm³)

Ozone Reaction:

No Ozone Reaction Estimation

Fraction sorbed to airborne particulates (phi):

1 (Junge-Pankow, Mackay avg)

0.915 (Koa method)

Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (KOCWIN v2.00):

*** WARNING: Inorganic Compound (Outside Estimation Domain) **

*** WARNING: Estimation NOT VALID **

Koc : 1.407 L/kg (MCI method)

Log Koc: 0.148 (MCI method)

Koc : 4.004 L/kg (Kow method)

Log Koc: 0.603 (Kow method)

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v2.00]:

Rate constants can NOT be estimated for this structure!

Bioaccumulation Estimates (BCFBAF v3.00):

Log BCF from regression-based method = 0.500 (BCF = 3.162 L/kg wet-wt)

Log Biotransformation Half-life (HL) = -2.0250 days (HL = 0.009441 days)

Log BCF Arnot-Gobas method (upper trophic) = -0.047 (BCF = 0.898)
 Log BAF Arnot-Gobas method (upper trophic) = -0.047 (BAF = 0.898)
 log Kow used: -0.77 (estimated)

Volatilization from Water:

Henry LC: 7.6E-015 atm-m3/mole (estimated by Bond SAR Method)
 Half-Life from Model River: 7.626E+010 hours (3.178E+009 days)
 Half-Life from Model Lake : 8.32E+011 hours (3.466E+010 days)

Removal In Wastewater Treatment:

Total removal: 1.85 percent
 Total biodegradation: 0.09 percent
 Total sludge adsorption: 1.76 percent
 Total to Air: 0.00 percent
 (using 10000 hr Bio P,A,S)

Removal In Wastewater Treatment:

Total removal: 75.06 percent
 Total biodegradation: 74.44 percent
 Total sludge adsorption: 0.62 percent
 Total to Air: 0.00 percent
 (using Biowin/EPA draft method)

Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.000587	611	1000
Water	37.3	360	1000
Soil	62.7	720	1000
Sediment	0.0704	3.24e+003	0

Persistence Time: 591 hr

ECOSAR Results for Phosphate:

SMILES : OP(=O)(O)O
 CHEM : PHOSPHATE
 CAS Num: 014265-44-2
 ChemID1:
 ChemID2:
 ChemID3:
 MOL FOR: H3 O4 P1
 MOL WT : 98.00
 Log Kow: -0.77 (KowWin estimate)
 Melt Pt:
 Wat Sol: 5.386E+005 mg/L (WskowWin estimate)

ECOSAR v1.00 Class(es) Found

 Neutral Organics

ECOSAR Class	Organism	Predicted		
		Duration	End Pt	mg/L (ppm)
Neutral Organics	: Fish	96-hr	LC50	20670.012
Neutral Organics	: Fish	14-day	LC50	19987.178
Neutral Organics	: Daphnid	48-hr	LC50	7739.504
Neutral Organics	: Green Algae	96-hr	EC50	1103.342

Neutral Organics	: Fish	30-day	ChV	1788.696
Neutral Organics	: Daphnid		ChV	578.554
Neutral Organics	: Green Algae		ChV	265.686
Neutral Organics	: Fish (SW)	96-hr	LC50	35468.875
Neutral Organics	: Mysid Shrimp	96-hr	LC50	1.49e+005
Neutral Organics	: Fish (SW)		ChV	612.736
Neutral Organics	: Mysid Shrimp (SW)		ChV	29203.973
Neutral Organics	: Earthworm	14-day	LC50	330.099

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect.

Neutral Organics:

 For Fish LC50 (96-h), Daphnid LC50, Mysid: If the log Kow is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

For Fish LC50 (14-day) and Earthworm LC50: If the log Kow is greater than 6.0, or if the compound is solid and the LC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

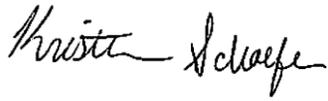
For Green Algae Acute Toxicity Values: If the log Kow of the chemical is greater than 6.4, or if the compound is solid and the EC50 exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

For All Chronic Toxicity Values: If the log Kow of the chemical is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

ECOSAR v1.00 SAR Limitations:

 Maximum LogKow: 5.0 (Fish 96-hr LC50; Daphnid LC50, Mysid LC50)
 Maximum LogKow: 6.0 (Fish 14-day LC50; Earthworm LC50)
 Maximum LogKow: 6.4 (Green Algae EC50)
 Maximum LogKow: 8.0 (ChV)
 Maximum Mol Wt: 1000

Melamine Polyphosphate Green Screen Evaluation Prepared By:



Kristen M. Schaefer, M.F.S.
Associate Toxicologist
ToxServices LLC

Melamine Polyphosphate Green Screen Evaluation QC'd By:



Margaret H. Whittaker, Ph.D., M.P.H., E.R.T., D.A.B.T.
Managing Director and Chief Toxicologist
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APPENDIX IX I: GREEN SCREEN FOR RED PHOSPHORUS (CAS #7723-14-0)²⁵

Also Called: Amgard CPC, Amgard CPC 405, Black phosphorus, Bonide blue death rat killer, Caswell No. 663, Common sense cockroach and rat preparations, EINECS 231-768-7, EPA Pesticide Chemical Code 066502, Exolit 385, Exolit 405, Exolit LPKN, Exolit LPKN 275, Exolit RP 605, Exolit RP 650, Exolit RP 652, Exolit RP 654, Exolit VPK-n 361, FR-T 2 (element), Gelber phosphor, Gelber phosphor [German], HSDB 1169, Hishigado, Hishigado AP, Hishigado CP, Hishigado NP 10, Hishigado PL, Hostaflam RP 602, Hostaflam RP 614, Hostaflam RP 622, Hostaflam RP 654, Masteret 70450, NVE 140, Nova Sol R 20, Novaexcel 140, Novaexcel 150, Novaexcel F 5, Novaexcel ST 100, Novaexcel ST 140, Novaexcel ST 300, Novared 120UF, Novared 120UFA, Novared 120VFA, Novared 140, Novared 280, Novared C 120, Novared F 5, Phosphorus, Phosphorus (red), Phosphorus-31, Rat-Nip, Red phosphorus, UNII-27YLU75U4W, Violet phosphorus, White Phosphorus

Chemical Structure of Red Phosphorus:

P

For Inorganic Chemicals:

Define Form & Physiochemical Properties

13. Particle size (e.g. silica of respirable size) – unknown
14. Structure (e.g. amorphous vs. crystalline) – Crystalline (O’Neil 2001)
15. Mobility (e.g. Water solubility, volatility) – 2.4 mg/L at 15°C; 4.1 mg/L at 25°C (ESIS 2000)

Identify Applications/Functional Uses: Flame retardant

Green Screen Rating²⁶: Red phosphorus was assigned a Green Screen Benchmark Score of 1 based on the High human acute toxicity (AT) and systemic toxicity (ST) as well as the High neurotoxicity (N), which is a priority effect (1d).

Green Screen (Version 1) Levels of Concern for Red Phosphorus														
Human – Tier 1					Human – Tier 2				Eco		Fate		Physical	
C	M	R/D	ED	N	AT	Cr	Sn	ST	AA	CA	P	B	Ex	F
L	L	L	nd	H	H	H	L	H	L	M	M	L	H	H

*Endpoints in italics were assigned using estimated values and professional judgment (Structure Activity Relationships).

²⁵ CPA recommends independent third-party validation of all Green Screen assessments. No independent third-party validation has been done for this assessment. Companies may not make marketing claims based on a Green Screen assessment that has not undergone an independent validation.

²⁶ For inorganic chemicals with low human and ecotoxicity across all hazard endpoints and low bioaccumulation, persistence alone will not be deemed problematic. Inorganic chemicals that are only persistent will be evaluated under the criteria for Benchmark 4.

Transformation Products and Ratings:

Identify relevant fate and transformation products (i.e., dissociation products, transformation products, valence states) and/or moieties of concern²⁷

Life Cycle Stage	Transformation Pathway	Transformation Products	CAS #	Green Screen Rating
	Possible product of phosphorus coming in direct contact with air and water.	Phosphine	7803-51-2	Present on the Red List of Chemicals as a possible neurotoxicant (CPA 2009).
End of Life	Combustion	Phosphorus acids	10294-56-1 and 13598-36-2	Not present on the Red List of Chemicals (CPA 2009).
End of Life	Combustion	Polyphosphoric acids	8017-16-1	Not present on the Red List of Chemicals (CPA 2009).
End of Life	Decomposition	Phosphorus oxides	Multiple	Not present on the Red List of Chemicals (CPA 2009).
	Reaction with Water	Hypophosphorous acid	6303-21-5	Not present on the Red List of Chemicals (CPA 2009).
	Reaction with Water	Phosphoric acid	7664-38-2	Not present on the Red List of Chemicals (CPA 2009).

*The above transformation products were screened against the CPA's table of Red List chemicals.

Introduction

Phosphorus exists in three main allotropic forms: white (sometimes called yellow phosphorus), black, and red (O'Neil 2001). Red phosphorus is a stable transformation form of the element phosphorus (Leisewitz 2000). Toxicity data for red phosphorus produced conflicting conclusions; not all studies stated specifically the allotrope of phosphorus being tested therefore the results varied widely. Red phosphorus is less toxic than the white allotrope however; most studies did not distinguish between the red and the white forms and only identified the compound as "phosphorus." In an effort to be conservative, all data, unless it specifically stated white phosphorus was used, was taken into consideration.

Red phosphorus is an additive flame retardant stabilized by wetting it with additives or by micro-encapsulation with phenol formaldehyde resins. Red phosphorus decomposes

²⁷ A moiety is a discrete chemical entity that is a constituent part or component of a substance. A moiety of concern is often the parent substance itself for organic compounds. For inorganic compounds, the moiety of concern is typically a dissociated component of the substance or a transformation product.

thermally above 400°C. Its mode of action involves forming a rigid, glassy carbonized layer on the polymer that consists mainly of polyphosphoric acid, which prevents the re-supply of flammable material in the gas phase. The oxygen required for the formation of the polyphosphoric acid is derived preferentially from the matrix (polymer or other material). This makes red phosphorus a highly effective flame retardant in materials with high oxygen content such as cellulose or other oxygen-containing plastics. A synergist is required in oxygen-free materials such as polyolefins or polystyrene. Impurities found in red phosphorus mainly stem from white phosphorus which ignites in the presence of air (up to 200 mg/kg red phosphorus).

Red phosphorus does not dissolve easily in water (Leisewitz 2000). Risks of environmental contamination with red phosphorus as a result of its use as a flame retardant is low, while inertial and micro-encapsulated red phosphorus do not pose a hazard to the environment. Oral ingestion of free RP is unlikely due to its degradability in the environment. Fumes can lead to irritations of the skin and mucous membranes. Lack of oxygen can lead to the formation of white phosphorus, also called yellow phosphorus, which can ignite in the presence of air. The National Institute for Occupational Safety and Health (NIOSH) has assigned red phosphorus an exposure limit of 0.1 mg/m³ (TWA) and an immediately dangerous to life or health value (IDLH) of 5 mg/m³ (Avogadro 2000). OSHA assigned red phosphorus a Permissible Exposure Limit (PEL) of 0.1 mg/m³ (Avogadro 2000).

Human Health – Tier 1

Carcinogenicity (C) Score: (H, M or L): L

Red phosphorus was assigned a score of Low for carcinogenicity because no basis for concern was identified.

- Red phosphorus is not listed as a known carcinogen by IARC, NTP, U.S. EPA, or CA Prop 65.

Mutagenicity (M) and Genotoxicity Score: (H, M or L): L

Red phosphorus was assigned a score of Low for mutagenicity and genotoxicity because data from animal studies suggests the chemical is not clastogenic.

- Female rats were exposed to red phosphorus/butyl rubber at 1,000 mg/m³ over a 2 week period. It was concluded the test substance was a weak clastogen. No other details of the study were provided (U.S. EPA 2010b).

Reproductive (R) and Developmental (D) Toxicity Score: (H, M or L): L

Red phosphorus was assigned a score of Low for reproductive and developmental toxicity because no basis for concern was identified.

- There are no data to suggest that a single inhalation exposure to red phosphorus would cause developmental or reproductive toxicity (no other data provided) (U.S. EPA 2010b).

Endocrine Disruption (ED) Score: (H, M or L): nd

- Red phosphorus is not listed as a potential endocrine disruptor on the EU Priority List of Suspected Endocrine Disruptors.
- Red phosphorus is not listed as a potential endocrine disruptor on the OSPAR List of Chemicals of Possible Concern.
- Red phosphorus is not listed as a potential endocrine disruptor on the Red List of Chemicals (CPA 2009).

Neurotoxicity (N) Score: (H, M or L): H

Red phosphorus was assigned a score of High for neurotoxicity based on it being listed as a potential neurotoxicant.

- Red phosphorus is classified as a developmental neurotoxicant (Grandjean and Landrigan 2006).
- Red phosphorus is listed as a potential neurotoxicant on the Red List of Chemicals (CPA 2009).

Human Health – Tier 2

Acute Mammalian (AT) Toxicity Score: (H, M or L): H

Red phosphorus was assigned a score of High for acute mammalian toxicity based on oral LD₅₀ values < 50 mg/kg-bw. Data is based on studies from two routes of exposure in four different species.

***Note:** Unless specifically noted, it is unclear if these LD₅₀ values apply to the red phosphorus or the white (more toxic) phosphorus.

- *Oral:* An LD₅₀ of 3.3 mg/kg was determined in the rat (Avogadro 2000).
- *Oral:* An LD₅₀ of 11.5 mg/kg was determined in the rat (ChemCAS 2004).
- *Oral:* An LD₅₀ of 4.8 mg/kg was determined in the mouse (Avogadro 2000).
- *Oral:* An LD₅₀ of 11.5 mg/kg was determined in the mouse (ChemCAS 2004).
- *Oral:* An LD₅₀ of 105 mg/kg was determined in the rabbit (ChemCAS 2004).
- *Oral:* An LD₅₀ of > 15,000 mg/kg-bw was determined for red phosphorus in the rat (ESIS 2000).
- *Oral:* A dosage of 0.66 mg/kg-bw (red phosphorus) did not kill rabbits or guinea pigs, but did induce cirrhosis-like symptoms (Hayes 1991).
- *Inhalation:* An LC₅₀ (1 hour exposure time) of 4.3 mg/L (red phosphorus) was determined in the rat (ESIS 2000).

Corrosion/ Irritation (Skin/ Eye) (Cr) Score: (H, M or L): H

Red phosphorus was assigned a score of High for corrosion and irritation based on animal studies that showed the chemical to cause injury to skin and eyes.

- *Dermal:* Prolonged or repeated contact may cause irritation and/or dermatitis (Avogadro 2000).
- *Dermal:* If contaminated with white phosphorus, contact may cause deep, slow healing burns (J.T. Baker 2008).
- *Ocular:* May cause corneal injury (Avogadro 2000).
- *Ocular:* If contaminated with white phosphorus, contact can cause severe irritation and burns (J.T. Baker 2008).

Sensitization (Sn) Score (Skin and Respiratory): (H, M or L): L

Red phosphorus was assigned a score of Low for sensitization because no basis for concern was identified.

- *Dermal*: Red phosphorus is not sensitizing to guinea pigs (ESIS 2000)

Systemic/ Organ (ST) Toxicity Score (includes organ effects and immunotoxicity) (H, M or L): H

Red phosphorus was assigned a score of High for systemic/organ toxicity based on evidence of adverse effects in humans.

- Red phosphorus targets the liver and kidneys (Avogadro 2000).
- Chronic exposure to red phosphorus can lead to necrosis of the jaw or “phossy-jaw” (Avogadro 2000).
- Chronic exposure to red phosphorus can lead to blood disorders and cardiovascular effects (J.T. Baker 2008).
- Persons with pre-existing skin disorders or eye problems, jaw/tooth abnormalities, or impaired liver, kidney or respiratory function may be more susceptible to the effects of red phosphorus (J.T. Baker 2008).
- Mice and rats were exposed to the smoke produced by ignition of a red phosphorus pyrotechnic composition, 1 hr/day, 5 days/week, at two different dose levels (actual doses not provided by the authors), together with controls. The mice received 180 exposures, while the rats received 200 exposures. Guinea pigs also underwent 200 exposures at the lower concentration, but all animals exposed at the higher concentration died during or immediately after the first dose. Growth of the test groups of mice and rats was depressed during the exposure period. Organ specific toxicity appeared not to be present in rats and was generally confined to the respiratory tract of the mice and the guinea pigs. A significantly higher proportion of the test group mouse lung showed aggregates of macrophages containing granules than was present in the control group. Severe congestion was observed in practically all the lung from the decedent high-dose group guinea pigs (Marrs 1989).

Ecotoxicity

Acute Aquatic (AA) Toxicity Score: (H, M or L): L

Red phosphorus was assigned a score of Low for acute aquatic toxicity based on LC₅₀ values greater than 100 mg/L.

- An LC₅₀ of 2,609 mg/L was identified in fish (96 hour) (U.S. EPA 2009).
- An LC₅₀ of 1,051 mg/L was identified in the daphnid (aquatic invertebrate, 48 hour) (U.S. EPA 2009).
- An EC₅₀ of 186 mg/L was identified in green algae (aquatic plant, 96 hour) (U.S. EPA 2009).

Chronic Aquatic (CA) Toxicity Score: (H, M or L): M

Red phosphorus was assigned a score of Moderate for chronic aquatic toxicity based on the risk phrase of R52/53,

- Red phosphorus was assigned the following Risk Phrase: R52/53- Harmful to aquatic organisms, may cause long-term adverse effects in the aquatic environment (ChemCAS 2004).
- A ChV of 233 mg/L was identified in fish (30 day) (U.S. EPA 2009).
- A ChV of 85 mg/L was identified in daphnid (U.S. EPA 2009).
- A ChV of 48 mg/L was identified in green algae (U.S. EPA 2009).

Environmental Fate

Persistence (P) Score: (vH, H, M, or L): M

Red phosphorus was assigned a score of Moderate for persistence based on a half-life in soil of 30 days and a half-life in water of 15 days.

- EPI Suite – BIOWIN model results indicate phosphorus readily biodegrades, and has a predicted degradation time of days to weeks. STP removal expected using BIOWIN/EPA Draft Method results indicate 96.32% total removal, with 50.88% due to biodegradation. Fugacity modeling predicts 1.86% partitioning to soil with a half-life of 30 days, and 42.3% partitioning to water with a half-life of 15 days (U.S. EPA 2010a).

Bioaccumulation (B) Score: (vH, H, M, or L): L

Red phosphorus was assigned a score of Low for bioaccumulation based on a BCF less than 500.

- BCFBAF predicts a bioconcentration factor (BCF) of 0.9181 and a log K_{ow} of -0.27 (U.S. EPA 2010a).

Physical Properties

Explosivity (Ex) Hazard Rating: (H, M or L): H

Red phosphorus was assigned a score of High for explosivity based on the risk phrase R16.

- Red phosphorus was assigned the following Risk Phrase: R16- Explosive when mixed with oxidizing substances (Avogadro 2000).
- Lack of oxygen can lead to the formation of white phosphorus which is explosive when in contact with air (Leisewitz 2000).

Flammability (F) Hazard Rating: (H, M or L): H

Red phosphorus was assigned a score of High for flammability based on the risk phrase R11.

- Red phosphorus was assigned the following Risk Phrase: R11- Highly flammable (Avogadro 2000, ChemCAS 2004, J.T. Baker 2008).

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EPI Suite Results: Red Phosphorus:

CAS Number: 7723-14-0

SMILES : P

CHEM : PHOSPHORUS

MOL FOR: H3 P1

MOL WT : 34.00

----- EPI SUMMARY (v4.00) -----

Physical Property Inputs:

Log Kow (octanol-water): -----

Boiling Point (deg C) : -----

Melting Point (deg C) : -----

Vapor Pressure (mm Hg) : -----

Water Solubility (mg/L): -----

Henry LC (atm-m³/mole) : -----

Log Octanol-Water Partition Coef (SRC):

*** WARNING: Inorganic Compound (Outside Estimation Domain)

Log Kow (KOWWIN v1.67 estimate) = -0.27

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPVP v1.43):

*** WARNING: Inorganic Compound (Outside Estimate Domain) ***

*** WARNING: Estimations NOT VALID ***

Boiling Pt (deg C): 468.18 (Adapted Stein & Brown method)

Melting Pt (deg C): 162.02 (Mean or Weighted MP)

VP(mm Hg,25 deg C): 2.33E+004 (Mean VP of Antoine & Grain methods)

VP (Pa, 25 deg C) : 3.11E+006 (Mean VP of Antoine & Grain methods)

MP (exp database): -133 deg C

BP (exp database): -87.7 deg C

VP (exp database): 2.93E+04 mm Hg (3.91E+006 Pa) at 25 deg C

Water Solubility Estimate from Log Kow (WSKOW v1.41):

*** WARNING: Inorganic Compound (Outside Estimation Domain)**

Water Solubility at 25 deg C (mg/L): 2.048e+005

log Kow used: -0.27 (estimated)

no-melting pt equation used

Water Sol (Exper. database match) = 3.3 mg/L (15 deg C)

Exper. Ref: KIRK-OTHMER; on-line (2005)

Water Sol Estimate from Fragments:

*** WARNING: Inorganic Compound (Outside Estimation Domain)***

*** WARNING: Wat Sol Estimation NOT Valid ***

Wat Sol (v1.01 est) = 60349 mg/L

ECOSAR Class Program (ECOSAR v1.00):

Class(es) found: Neutral Organics

Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:

*** WARNING: Inorganic Compound (Outside Estimation Domain) **

*** WARNING: Estimation NOT VALID **

Bond Method : 2.44E-002 atm-m³/mole (2.48E+003 Pa-m³/mole)

Group Method: Incomplete

For Henry LC Comparison Purposes:

User-Entered Henry LC: not entered

Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:

HLC: 1.660E-004 atm-m³/mole (1.682E+001 Pa-m³/mole)

VP: 2.33E+004 mm Hg (source: MPBPVP)
WS: 2.05E+005 mg/L (source: WSKOWWIN)

Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1.10]:
*** WARNING: Inorganic Compound (Outside Estimation Domain)**
*** WARNING: Estimation NOT VALID ***
Log Kow used: -0.27 (KowWin est)
Log Kaw used: -0.001 (HenryWin est)
Log Koa (KOAWIN v1.10 estimate): -0.269
Log Koa (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10):
*** WARNING: Inorganic Compound (Outside Estimation Domain)**
*** WARNING: Estimation NOT VALID ***
Biowin1 (Linear Model) : 0.7314
Biowin2 (Non-Linear Model) : 0.9259
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model): 3.1240 (weeks)
Biowin4 (Primary Survey Model) : 3.7987 (days)
MITI Biodegradation Probability:
Biowin5 (MITI Linear Model) : 0.6110
Biowin6 (MITI Non-Linear Model): 0.8241
Anaerobic Biodegradation Probability:
Biowin7 (Anaerobic Linear Model): 0.8361
Ready Biodegradability Prediction: YES

Hydrocarbon Biodegradation (BioHCwin v1.01):
Structure incompatible with current estimation method!

Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
Vapor pressure (liquid/subcooled): 3.91E+006 Pa (2.93E+004 mm Hg)
Log Koa (Koawin est): -0.269
Kp (particle/gas partition coef. (m3/ug)):
Mackay model : 7.68E-013
Octanol/air (Koa) model: 1.32E-013
Fraction sorbed to airborne particulates (phi):
Junge-Pankow model : 2.77E-011
Mackay model : 6.14E-011
Octanol/air (Koa) model: 1.06E-011

Atmospheric Oxidation (25 deg C) [AopWin v1.92]:
*** WARNING: Inorganic Compound (Outside Estimation Domain)**
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant = 0.0000 E-12 cm3/molecule-sec
Half-Life = -----
Ozone Reaction:
No Ozone Reaction Estimation
Fraction sorbed to airborne particulates (phi):
4.46E-011 (Junge-Pankow, Mackay avg)
1.06E-011 (Koa method)
Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (KOCWIN v2.00):
*** WARNING: Inorganic Compound (Outside Estimation Domain) **
*** WARNING: Estimation NOT VALID **
Koc : 13.22 L/kg (MCI method)
Log Koc: 1.121 (MCI method)

Koc : 0.5825 L/kg (Kow method)
Log Koc: -0.235 (Kow method)

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v2.00]:
Rate constants can NOT be estimated for this structure!

Bioaccumulation Estimates (BCFBAF v3.00):

Log BCF from regression-based method = 0.500 (BCF = 3.162 L/kg wet-wt)
Log Biotransformation Half-life (HL) = -1.7075 days (HL = 0.01961 days)
Log BCF Arnot-Gobas method (upper trophic) = -0.037 (BCF = 0.9181)
Log BAF Arnot-Gobas method (upper trophic) = -0.037 (BAF = 0.9181)
log Kow used: -0.27 (estimated)

Volatilization from Water:

Henry LC: 0.0244 atm-m³/mole (estimated by Bond SAR Method)
Half-Life from Model River: 0.609 hours (36.54 min)
Half-Life from Model Lake : 55.54 hours (2.314 days)

Removal In Wastewater Treatment:

Total removal: 90.47 percent
Total biodegradation: 0.02 percent
Total sludge adsorption: 0.39 percent
Total to Air: 90.06 percent
(using 10000 hr Bio P,A,S)

Removal In Wastewater Treatment (recommended maximum 95%):

Total removal: 96.32 percent
Total biodegradation: 50.88 percent
Total sludge adsorption: 0.27 percent
Total to Air: 45.18 percent
(using Biowin/EPA draft method)

Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	55.7	1e+005	1000
Water	42.3	360	1000
Soil	1.86	720	1000
Sediment	0.101	3.24e+003	0

Persistence Time: 146 hr

ECOSAR Results: Red Phosphorus:

SMILES : P
CHEM : PHOSPHORUS
CAS Num: 007723-14-0
ChemID1:
ChemID2:
ChemID3:
MOL FOR: H3 P1
MOL WT : 34.00
Log Kow: -0.27 (KowWin estimate)
Melt Pt:
Wat Sol: 3.3 mg/L (experimental database)

ECOSAR v1.00 Class(es) Found

 Neutral Organics

ECOSAR Class	Organism	Predicted		
		Duration	End Pt	mg/L (ppm)
Neutral Organics	: Fish	96-hr	LC50	2609.779 *
Neutral Organics	: Fish	14-day	LC50	2543.939 *
Neutral Organics	: Daphnid	48-hr	LC50	1051.975 *
Neutral Organics	: Green Algae	96-hr	EC50	186.249 *
Neutral Organics	: Fish	30-day	ChV	233.517 *
Neutral Organics	: Daphnid		ChV	85.106 *
Neutral Organics	: Green Algae		ChV	48.739 *
Neutral Organics	: Fish (SW)	96-hr	LC50	4311.682 *
Neutral Organics	: Mysid Shrimp	96-hr	LC50	13151.021 *
Neutral Organics	: Fish (SW)		ChV	103.053 *
Neutral Organics	: Mysid Shrimp (SW)		ChV	2228.113 *
Neutral Organics	: Earthworm	14-day	LC50	101.661 *

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect.

Neutral Organics:

 For Fish LC50 (96-h), Daphnid LC50, Mysid: If the log Kow is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

For Fish LC50 (14-day) and Earthworm LC50: If the log Kow is greater than 6.0, or if the compound is solid and the LC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

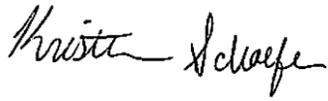
For Green Algae Acute Toxicity Values: If the log Kow of the chemical is greater than 6.4, or if the compound is solid and the EC50 exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

For All Chronic Toxicity Values: If the log Kow of the chemical is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

ECOSAR v1.00 SAR Limitations:

 Maximum LogKow: 5.0 (Fish 96-hr LC50; Daphnid LC50, Mysid LC50)
 Maximum LogKow: 6.0 (Fish 14-day LC50; Earthworm LC50)
 Maximum LogKow: 6.4 (Green Algae EC50)
 Maximum LogKow: 8.0 (ChV)
 Maximum Mol Wt: 1000

Red Phosphorus Green Screen Evaluation Prepared By:



Kristen Schaefer, M.F.S.
Associate Toxicologist
ToxServices LLC

Red Phosphorus Green Screen Evaluation QC'd By:

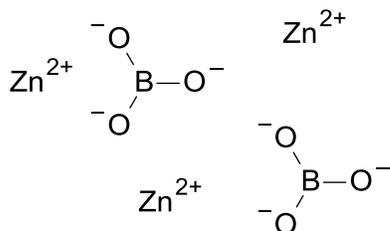


Margaret H. Whittaker, Ph.D., M.P.H., E.R.T., D.A.B.T.
Managing Director and Chief Toxicologist
ToxServices LLC

APPENDIX IX J: GREEN SCREEN FOR ZINC BORATE (CAS #1332-07-6)²⁸

Also Called: Alcanex FR 100, Alcanex FRC 600, Bonrex FC, Borax 2335, Boric acid, zinc salt, Climax ZB 467, EINECS 215-566-6, EPA Pesticide Chemical Code 128859, FRC 600, Flamtard Z 10, HSDB 1046, JS 9502, SZB 2335, XPI 187, ZB 112, ZB 237, ZB 467 Lite, ZN 100, ZSB 2335, ZT, ZT (fire retardant), Zinc borate

Chemical Structure of Zinc Borate:



***Note:** Data gaps for this chemical were addressed by evaluating the toxicity data on zinc oxide (CAS #1314-13-2) and boric acid (CAS #10043-35-3; 11113-50-1). ToxServices selected these chemicals as they are degradation products of the parent compound and structurally similar to the parent compound.

For Inorganic Chemicals:

Define Form & Physiochemical Properties

16. Particle size (e.g. silica of respirable size) – 8-20 μ m particle size (e.g. silic)
17. Structure (e.g. amorphous vs. crystalline) – n/a
18. Mobility (e.g. Water solubility, volatility) – 0.1% at pH 5 and 7, and 0.03% at pH 9 (U.S. EPA 1991)

Identify Applications/Functional Uses: Flame retardant.

Green Screen Rating²⁹: Zinc borate was assigned a Benchmark Score of 2 based on a Moderate hazard rating for reproductive and developmental (R/D) toxicity (1d).

Green Screen (Version 1.0) Levels of Concern for Zinc Borate														
Human – Tier 1					Human – Tier 2				Eco		Fate		Physical	
C	M	R/D	ED	N	AT	Cr	Sn	ST	AA	CA	P	B	Ex	F
L	L	<i>M</i>	<i>M</i>	nd	L	M	L	M	H	nd	nd	L	L	L

*Endpoints in italics were assigned using estimated values and professional judgment (Structure Activity Relationships).

²⁸ CPA recommends independent third-party validation of all Green Screen assessments. No independent third-party validation has been done for this assessment. Companies may not make marketing claims based on a Green Screen assessment that has not undergone an independent validation.

²⁹ For inorganic chemicals with low human and ecotoxicity across all hazard endpoints and low bioaccumulation, persistence alone will not be deemed problematic. Inorganic chemicals that are only persistent will be evaluated under the criteria for Benchmark 4.

Transformation Products and Ratings:

Identify relevant fate and transformation products (i.e., dissociation products, transformation products, valence states) and/or moieties of concern³⁰

Life Cycle Stage	Transformation Pathway	Transformation Products	CAS #	Green Screen Rating
End of Life	Dissociation	Zinc, cation	23713-49-7	Not present on the Red List of Chemicals (CPA 2009)
End of Life	Dissociation	Borate, anion	39201-27-9	Not present on the Red List of Chemicals (CPA 2009)
End of Life	Degradation	Zinc oxide	1314-13-2	Not present on the Red List of Chemicals (CPA 2009)
End of Life	Degradation	Boric acid	10043-35-3; 11113-50-1	Endocrine Disruptor (CPA 2009)

*The above transformation products were screened against the CPA's table of Red List chemicals (CPA 2009).

Introduction

Zinc borate is used as a flame retardant in conjunction with other chemicals, including antimony trioxide, magnesium hydroxide, alumina trihydrate, and some brominated flame retardants. Zinc borate is used as a flame retardant on commercial furniture, draperies, wall coverings, and carpets (R.C.Kidder, Flame Retardant Chemical Association, unpublished material, April 21, 1998). In addition, zinc borate is used as a fungicide (NAS 2000).

A literature search identified limited publications relating to the toxicity of zinc borate. However, variety of toxicological studies have been performed on various inorganic borates. Longer-term toxicological studies have been reported, and are mainly on boric acid or borax. There is similarity in the toxicological effects of boric acid and borax across different animal species (Hubbard 1998).

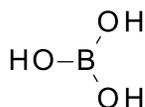
Additionally, zinc borate readily breaks down in the stomach to zinc oxide (ZnO) and boric acid (H₃BO₃) (NAS 2000). Therefore, in the absence of data for zinc borate, the data for zinc oxide and boric acid will be substituted. Zinc oxide is used as a pigment in paint, cosmetics, and dental and quick drying cements. Therapeutically, zinc oxide is

³⁰ A moiety is a discrete chemical entity that is a constituent part or component of a substance. A moiety of concern is often the parent substance itself for organic compounds. For inorganic compounds, the moiety of concern is typically a dissociated component of the substance or a transformation product.

used as an astringent and as a topical protectant. Boric acid is used in enamels, porcelain, soaps, cosmetics, and as an insecticide. Therapeutically, boric acid is used as an astringent and an antiseptic (NAS 2000).

The critical health effect endpoints in several species are male reproductive toxicity and developmental toxicity. Humans would need to consume daily doses of 3.3 g of boric acid (or 5.0 g borax) to ingest the same dose level as the lowest animal NOAEL. No effects on fertility were seen in a population of workers exposed to borates or to a population exposed to high environmental borate levels (Hubbard 1998).

Chemical Structure of Surrogates



Boric Acid (CAS #10043-35-3; 11113-50-1)



Zinc Oxide (CAS #1314-13-2)

Human Health – Tier 1

Carcinogenicity (C) Score (H, M or L): L

Because carcinogenicity data were unavailable for zinc borate, the structurally similar zinc oxide and boric acid were used as surrogates. Zinc borate was assigned a score of Low for carcinogenicity based on negative results from surrogate studies.

Zinc borate

- Not listed as a known carcinogen by IARC, NTP, U.S. EPA, or CA Prop 65.

Zinc oxide

- Not classifiable as to human carcinogenicity due to inadequate evidence in humans and animals (U.S. EPA 2005).

Boric acid

- In long term feeding studies on boric acid and disodium tetraborate decahydrate in both rats and dogs, no carcinogenic effects were observed (Weir and Fisher 1972). In rats, diets contained disodium tetraborate decahydrate or boric acid at 0, 117, 350, and 1,170 ppm boron equivalents for 2 years; these doses were approximately 0, 5.9, 17.5 or 58.5 mg B/kg bw/day. Effects observed in these rat studies included lowered food consumption, retarded body weight gain, course hair coats, haunched position, swollen pads, inflamed bleeding eyes and changes in haematological parameters at the highest doses (58.5 mg B/kg bw/day). Dogs were fed diets containing boric acid (0.033%, 0.067%, 0.2% in diet) or disodium tetraborate decahydrate at (0.051%, 0.103%, 0.309%). No evidence of toxicity was observed. Therefore, additional groups of dogs (4 male and 4 female) were fed diets containing 0.67% boric acid or 1.03% disodium tetraborate decahydrate. The estimated equivalent boron intakes from the boric acid diet were 1.7, 3.8, 10.9 and 40.8 mg B/kg bw/day and from the disodium tetraborate decahydrate diet were 1.9, 3.6, 9.6 and 38.1 mg B/kg bw/day. In dogs, diarrhea was observed in some and soft stools in all dogs at the highest dose tested. Testicular effects

were observed in both rats and dogs. Testicular atrophy with some interstitial cell hyperplasia was the critical effect seen in a US National Toxicology Program (NTP) bioassay in mice (dose levels in food 0, 2,500, 5,000 ppm boric acid). No carcinogenic effects were observed at these doses estimated to be equivalent to 78 mg B/kg bw/day and 201 mg B/kg bw/day (NTP 1987). Effects on survival rate and reduced body weight gain were seen at the high doses. The studies carried out are not to modern standards, nor to GLP. However, they are well performed and reported, and are more than adequate to evaluate the carcinogenicity of boric acid and sodium tetraborates. It can be concluded that boric acid and sodium tetraborates are not carcinogenic and there is no concern for a carcinogenic effects in humans (HERA 2005).

Mutagenicity (M) and Genotoxicity Score (H, M or L): L

Because mutagenicity and genotoxicity data for zinc borate are limited, additional data for zinc oxide and boric acid are included. Zinc borate was assigned a score of Low for mutagenicity and genotoxicity based on negative mutagenicity results.

Zinc borate

- Zinc borate did not induce either genotoxic effects or chromosomal aberrations in mutagenicity studies (U.S. EPA 1991).
- In the Salmonella/microsomal assay (Ames assay) for bacterial mutagenic activity, zinc borate did not elicit any mutagenic response in *Salmonella* tester strains when tested either with or without a metabolic activation system (the EPA did not identify specific strains or concentrations) (U.S. EPA 1991).

Zinc oxide

- Several studies were identified that investigated the genotoxicity of zinc oxide. Data on other zinc compounds are relevant for a hazard evaluation based on the assumption that after intake the biological activities of zinc compounds are determined by the zinc cation. Available data indicate that the genotoxicity results vary widely. Conflicting results have been found, even in the same test systems. Overall, the results of the *in vitro* tests indicate that zinc has genotoxic potential. This is based on positive results in mammalian test systems for gene mutations and chromosomal aberrations as well as on the positive *in vitro* UDS test. *In vivo* increases in chromosomal aberrations were found in calcium-deficient mice exposed via the diet as well as in mice with normal calcium status when dosed intraperitoneally. Additionally, negative results were obtained in mice at higher intraperitoneal dose levels. Rats tested negative for chromosomal aberrations after oral dosing, either via gavage or via the diet. The positive result for chromosomal aberrations *in vitro* is considered overruled by negative *in vivo* tests for this endpoint. The positive sperm head abnormality test is considered sufficiently counter-balanced by two negative SLRL tests as well as two negative dominant lethal tests. Moreover, this sperm test is not adequately reported and without details on scoring criteria, interpretation of the observations is rather subjective. In addition, sperm head abnormalities are indicative rather than proof for genotoxicity. Based on the available data there is insufficient ground to classify zinc as genotoxic. It should be noted that the potential to induce gene mutations was not adequately tested *in vivo*. However, there is no clear evidence from the available data that zinc is genotoxic *in vivo* and, without a clear

indication for carcinogenicity, guidance for further testing with respect to target tissue is not available (ESIS 2008).

Boric acid

- A number of *in vitro* mutagenicity studies, including bacterial mutation assays in *Salmonella typhimurium* and *Escherichia coli*, gene mutation in mammalian cells (L5178Y mouse lymphoma, V79 Chinese hamster cells, C3H/10T1/2 cells), bacterial DNA-damage assay, unscheduled DNA synthesis (hepatocytes), chromosomal aberration and sister chromatid exchange in mammalian cell (Chinese hamster ovary, CHO cells) have been carried out on boric acid, disodium tetraborate decahydrate or disodium octaborate tetrahydrate. No evidence of mutagenic activity was observed (NTP 1987; Haworth et al. 1983; Landolph 1985; Bakke 1991; Stewart 1991).
- No mutagenic activity was seen *in vivo* in a mouse bone marrow micronucleus study on boric acid (O'Loughlin 1991).

Reproductive (R) and Developmental (D) Toxicity Score (H, M or L): M

Because reproductive and developmental toxicity data were unavailable for zinc borate, the structurally similar zinc oxide and boric acid were used as surrogates. Zinc borate was assigned a score of Moderate for reproductive and developmental toxicity based on developmental effects reported in rats, mice and rabbits exposed to boric acid (H_3BO_3). The most sensitive species appears to be rats, in which the effects observed at non-maternally toxic doses include a reduction in fetal body weight and minor skeletal variations.

Zinc borate

- No relevant reproductive and developmental toxicity data were identified for zinc borate.

Zinc oxide

- Groups of Sprague-Dawley rats (10/group) were fed diets containing 2,000 or 5,000 mg ZnO/kg feed (calculated to be 150 or 375 mg ZnO/kg bw [≈ 120 or 300 mg Zn^{2+} /kg bw/day]) from day 0 of gestation to day 14 of lactation, then mothers and remaining pups were killed. The control animals received a basal diet containing 9 mg Zn^{2+} /kg feed. Maternal weight, daily food intake, duration of gestation, and the number of viable young/litter were not affected. No external malformations were seen. Two females at 5,000 mg/kg feed had all stillborn litters containing edematous pups. At 2,000 mg/kg feed, 4 stillborn pups (not edematous) were observed. Dry liver weights of pups (newborn and 14 days old) were decreased at 5,000 mg/kg feed. A dose-related increase in zinc content and a dose-related decrease in iron content were observed. The livers of newborns of zinc-treated dams, however, contained significantly more iron than the controls. This was not observed in the 14-day old pups. The copper levels in the liver were significantly lower only in the newborns of the 5,000 mg/kg level. After 14 days the copper concentrations were significantly lower in all treated pups (Ketcheson et al. 1969).
- Bleavins et al. (1983) exposed groups of mink (11 females and 3 males/group) to a basal diet (containing 20.2 mg Zn^{2+} /kg diet and 3.1 mg Zn^{2+} /kg diet) or to the diet supplemented with 1,000 mg ZnO/kg diet. No maternal effects were seen. All females on the basal diet produced offspring, 8/11 females of the Zn-

supplemented diet group had young. None of the animals (males, females and kits) were sacrificed, so they were only macroscopically examined. The kits were kept on the basal and supplemented diets. The body weight of male kits on the supplemented diet was significantly lower at 12 weeks of age. 8-Week old kits on the supplemented diet showed a significant decrease of the Ht-value, the other blood parameters were comparable to the kits on basal diet. The decreased T-cell mitotic response observed in the Zn-supplemented kits was reversible when the kits were placed on basal diet. Kits (3-4 weeks old) of females fed the Zn-supplemented diet showed effects consistent with copper deficiency, such as grey fur around eyes, ears, jaws and genitals together with hair loss and dermatosis in these areas.

- Hence, with respect to effects on reproduction, zinc deficiency is known to result in impairment of fertility and of fetal development. In humans additional zinc up to 0.3 mg Zn²⁺/kg bw/day during pregnancy did not result in adverse effects. Available data in animals on zinc excess indicate that adverse effects on fertility and fetal development may occur at dose levels of 200 mg Zn²⁺/kg bw/day, in conjunction with other effects such as perturbation of parental and fetal copper homeostasis. In humans, a small disturbance (if any) of normal physiology, presumably indicative for copper deficiency, has been demonstrated at zinc excess of 50 and 150 mg Zn²⁺/day (0.83 and 2.5 mg Zn²⁺/kg bw/day, respectively), while 150 mg Zn²⁺/day (2.5 mg Zn²⁺/kg bw/day) resulted in clinical signs. As the margin between the dose at which in humans clinical signs are manifested and the dose at which in animals reproductive effects have been reported is so high (viz. 80), it is considered unlikely that in humans reproductive effects will occur at exposure levels at which clinical signs are not manifest. Therefore, neither fertility nor developmental toxicity is considered end-points of concern for humans. Based on the available information there is no reason to classify metallic zinc nor any of the zinc compounds considered for reproductive toxicity.

Boric acid

- Effects on the testis have been observed in both sub-chronic and chronic studies in three species: rats, mice and limited studies in dogs. In rats, a single dose of 175 mg B/kg bw was found to cause reversible disruption of tubular spermiation (Linder et al. 1990), although no such effects were observed after a single dose of 350 mg B/kg (2,000 mg boric acid/kg) (Bouissou and Castagnol 1965). The effects tend to be similar in all three species, although most data comes from rat studies. The reproductive effects in rats at lower doses and shorter time periods start with reversible inhibition of spermiation. Early effects were seen after 14 days treatment, at doses around 39 mg B/kg, (217 mg boric acid/kg bw/day) but at a lower dose of 26 mg B/kg (149 mg boric acid/kg bw/day) the effects take about 28 days to manifest (Ku et al. 1993). In a rat three generation study of boric acid and disodium tetraborate decahydrate, doses equivalent to 58.5 mg B/kg bw/day led to testicular atrophy, degeneration of seminiferous tubules, reduced sperm count and a reduction in fertility, with a NOAEL of 17.5 mg B/kg bw/day (Weir and Fisher 1972). Similar results were seen in a two-year study of boric acid and disodium tetraborate decahydrate at 58.5 mg B/kg bw/day where the NOAEL was also 17.5 mg B/kg bw/day (Weir and Fisher 1972). In male rats fed disodium

- tetraborate decahydrate for either 30 or 60 days at 100 or 200 mg B/kg bw/day testis weight was reduced, testicular germ cells were depleted, selected testicular enzymes were affected and fertility was reduced. The NOAEL was 50 mg B/kg bw/day (Lee et al. 1978). As might be expected, while recovery from inhibition of spermiation occurred at the lower doses, there was no recovery from testicular atrophy when the germ cells were lost.
- Data in dogs derives from two very limited and unreliable two-year dietary studies. Unfortunately, the published study does not accurately reflect the original study reports (Weir and Fisher 1972). In the published paper, the authors estimated the dietary intakes from standard intake figures. However, actual dietary intake was reported in the original study reports allowing a more accurate measure of the dietary intake to be made which are used in this review. Groups of only four male dogs were fed either boric acid or disodium tetraborate decahydrate at doses up to 10.2 mg B/kg bw/day (62.4 mg boric acid/kg bw/day and 84.7 mg disodium tetraborate decahydrate/kg bw/day) in one study and 39.5 mg B/kg bw/day (233.1 mg boric acid/kg bw/day and 373.2 mg disodium tetraborate decahydrate/kg bw/day) in a second study. The animals were sacrificed at various time periods such that observations were reported on only 1 or 2 animals. At 39.5 mg B/kg bw/day, testicular atrophy was observed, however the effects in the only one disodium tetraborate decahydrate treated dog investigated at 38 weeks were less severe than those seen in the control dog. Also, testicular atrophy was present in three out of four control dogs, so that the significance of the effect in the treated animals is difficult to assess. One boric acid treated and one disodium tetraborate decahydrate treated dog were allowed to recover for three weeks. Some recovery was observed in each dog. Minor histopathological changes such as decreased spermatogenesis remained which was less obvious in the disodium tetraborate decahydrate treated dog. The NOAEL was deemed to be the equivalent of 10.2 mg B/kg bw/day by the authors (Weir 1966 a,b; 1967 a,b; Weir and Fisher 1972). For the reasons given above (effects in control animals, insufficient group sizes, inaccurate dose reporting), this data is not reliable for risk assessment, but it does confirm the effects seen in other species. Due to the acute toxic effects of borates in dogs, had the LOAEL doses been administered as a single dose (i.e. by gavage) then vomiting would have occurred and the study would not have been possible.
 - A dose-related effect on the testis was observed in rats and mice with confirmation from limited and unreliable studies in dogs. Effects start with reversible inhibition of spermiation after 14 days treatment, at doses around 39 mg B/kg, (217 mg boric acid/kg bw/day) although at a lower dose of 26 mg B/kg (149 mg boric acid/kg bw/day) the effects take about 28 days to manifest. Higher doses (58.5 mg B/kg bw/day and above) led to testicular atrophy, degeneration of seminiferous tubules, reduced sperm count and a reduction in fertility. No recovery from testicular atrophy was observed when the germ cells were lost. The NOEL for this endpoint is 17.5 mg B/kg corresponding to 100 mg boric acid/kg/day; 155 mg disodium tetraborate decahydrate/kg and 118 mg disodium tetraborate pentahydrate/kg (HERA 2005).
 - The majority of developmental toxicity studies have been carried out in rats exposed to boric acid (H₃BO₃). In two separate dietary studies performed in the

same laboratory, groups of rats were given dose levels of approximately 3.3, 6.3, 9.6, 13.7, 25, 28 and 59 mg B/kg bw/day on gestation days 0-20 and 94 mg B/kg bw/day on gestation days 6-15 in feed. The NOAELs for maternal toxicity and developmental effects were 13.7 mg/kg bw/day and 9.6 mg B/kg bw/day (equivalent to 54.9 mg H₃BO₃/kg-bw)³¹, respectively. A reduction in food intake and an increase in relative liver and kidney weight and a reduction in maternal body weight gain at higher doses indicated maternal toxicity. At non-maternally toxic doses, there was a reduction on fetal weight and some skeletal variations and malformations (increase in wavy ribs and short rib XIII and a decreased incidence of rudimentary extra rib on lumbar 1), which had reversed by postnatal day 21 at 13.7 mg B/kg bw/day also, with the exception of short rib XIII, had reversed at 28.6 mg B/kg bw/day in a study designed to look at postnatal recovery (Price et al. 1990, 1996). At higher maternally toxic doses, other indications of developmental effects were observed, including resorptions and visceral malformations (enlarged lateral ventricles; cardiovascular effects; anophthalmia and microphthalmia and short and curly tails). However, these are likely to have been secondary to the maternal toxicity (Price et al. 1990, 1996; Heindel et al. 1992).

- Similar findings were observed in mice receiving estimated doses of 0, 43, 79, and 175 mg B/kg bw/day on gestation days 0-20 in feed. Maternal toxicity was indicated by a dose related incidence of renal tubule dilation/regeneration and at the highest dose increases food and water consumption in late gestation and in the relative kidney weight. A NOAEL was not determined for maternal toxicity. The key developmental effects observed were similar to those seen in rats i.e. a reduction in foetal body weight at the mid dose (79 mg B/kg) and an increase in skeletal variations and malformations (missing lumbar vertebrae, fused vertebral arches and short rib XIII) and resorptions at the highest, more maternally toxic dose. The NOAEL for developmental effects in mice was 43 mg B/kg bw/day (Heindel et al. 1992); however, this dose was also a maternally toxic dose.
- In rabbits receiving estimated doses of 0, 11, 22 and 44 mg B/kg bw/day by gavage on gestation days 6-19 maternal toxicity was indicated by effects such as an increase in relative kidney weight, increase food intake, vaginal bleeding and an increase in corrected weight gain. Developmental effects were seen only at the top dose, where the majority of the embryos were resorbed and malformations were primarily visceral (major heart and/or great vessel defects); however, these effects are likely to be secondary to the maternal toxicity. The only skeletal effect observed was a decreased incidence of rudimentary extra rib on lumbar 1 which was not considered biologically significant. The NOAEL for both maternal and developmental toxicity in the rabbit was 21.8 mg B/kg bw/day (Price et al. 1991).
- Developmental effects have been observed in three species, rats, mice and rabbits. The most sensitive species appears to be rats, in which the effects observed at non-maternally toxic doses include a reduction in fetal body weight and minor skeletal variations which, with the exception of short rib XIII, had reversed by 21

³¹ $\frac{9.6 \text{ mg B}}{\text{kg bw}} * \frac{\text{g B}}{1,000 \text{ mg B}} * \frac{\text{mol B}}{10.811 \text{ g B}} * \frac{\text{mol H}_3\text{BO}_3}{\text{mol B}} * \frac{61.83302 \text{ g H}_3\text{BO}_3}{\text{mol H}_3\text{BO}_3} * \frac{1,000 \text{ mg H}_3\text{BO}_3}{\text{g H}_3\text{BO}_3} = 54.9 \frac{\text{mg H}_3\text{BO}_3}{\text{kg bw}}$

days post natal. The NOAEL for developmental effects is 9.6 mg B/kg (HERA 2005).

Endocrine Disruption (ED) Score (H, M or L): M

Because endocrine disruption data were unavailable for zinc borate, the structurally similar zinc oxide and boric acid were used as surrogates. Zinc borate was assigned a score of Moderate for endocrine disruption based on suggestive animal studies for boric acid and the presence of boric acid on the European Union Priority List of Suspected Endocrine Disruptors.

Zinc borate

- Not listed as a potential endocrine disruptor on the EU Priority List of Suspected Endocrine Disruptors.
- Not listed as a potential endocrine disruptor on the OSPAR List of Chemicals of Possible Concern.
- Not listed as a potential endocrine disruptor on the Red List of Chemicals (CPA 2009).

Zinc oxide

- No relevant data were identified.

Boric acid

- The majority of toxicological studies have been reported on boric acid (H_3BO_3) or disodium tetraborate, known as borax ($Na_2B_4O_7 \cdot 10H_2O$). The inorganic borates display low acute toxicity orally, dermally or by inhalation. They are either not irritant or mild skin and eye irritants. They are not skin sensitizers, nor are they mutagenic or carcinogenic. In sub acute and chronic studies of boric acid in rats, mice, and dogs, the target organ is the testis. Effects on reproductive organs in females were seen, but at higher doses than in males. Effects on fertility were also seen in rats in a three-generation study and in mice in a continuous breeding study. The testicular effects observed include reduction in sperm count, inhibition of spermiation, and testicular atrophy. Reversal of inhibition of spermiation and reduced sperm count in rats was seen after removal of treatment at 38 mg B/kg bw/day (equivalent to 217 mg/kg bw/day boric acid). Minimal inhibition of spermiation was observed at 26 mg B/kg bw/day. A dose of 17 mg B/kg bw/day in male rats (equivalent to 97 mg/kg bw/day boric acid) was the NOAEL. Developmental toxicity has also been demonstrated in mice, rats and rabbits, with rats the most sensitive species. Administration of a wide range of doses of boric acid to pregnant rats for the whole of gestation has shown that at doses of 330 mg/kg bw/day (equivalent to 58 mg B/kg bw/day) and above, there is a high resorption rate and retardation of fetal development. At a lower dose of 28 mg B/kg bw/day, the only effects observed were reduced fetal weight and short 13th rib and wavy rib. These effects disappear if the pups are allowed to be delivered and reared to weaning. The NOAEL was 9.6 mg B/kg bw/day (equivalent to 54 mg/kg bw/day boric acid) (Hubbard 1995).
- To assess whether or not male reproductive toxicity can be evaluated in a 2 week administration study, boric acid was administered daily by oral gavage to male Jcl:Wistar rats at dosage levels of 0, 300, and 500 mg/kg for 2 and 4 weeks, and the results obtained with the 2 different treatment schedules were compared. After a 2 week administration, decreased testis weights were observed in the 500

mg/kg group. Histopathologically, exfoliation of round spermatids, retention of step 19 spermatids, and increased numbers of residual body-like structures in the seminiferous tubules and cell debris in the cranial epididymal ducts were observed in the 300 and 500 mg/kg groups. Distorted cytoplasmic lobes of step 19 spermatids, debris in the seminiferous tubules, and focal atrophy of the seminiferous tubules with multinucleated giant cells formation and necrosis of spermatocytes were also observed in the 500 mg/kg group. After a 4 week administration, testis and epididymis weights were decreased in the 300 and 500 mg/kg groups. Histopathological changes in the 300 mg/kg group were similar to those found in the 300 and 500 mg/kg groups after a 2 week administration. Diffuse atrophy of the seminiferous tubules was additionally observed in the 500 mg/kg group. These results suggest that 2 week is a sufficient treatment period for the detection of the testicular toxicity caused by boric acid (Fukuda et al. 2000).

Neurotoxicity (N) Score (H, M or L): nd

Because neurotoxicity data were unavailable for zinc borate, the structurally similar zinc oxide and boric acid were used as surrogates. No relevant neurotoxicity data were identified for zinc borate, zinc oxide, or boric acid.

Zinc borate

- Not classified as a developmental neurotoxicant (Grandjean and Landrigan 2006).
- Not listed as a potential neurotoxicant on the Red List of Chemicals (CPA 2009).

Zinc oxide

- Special studies were conducted to examine the morphological and histoenzymatic changes of the brain. Twelve Wistar rats were given daily doses of 100 mg ZnO (ca. 600 mg ZnO/kg bw \approx 480 mg Zn²⁺/kg bw) intragastrically for 10 consecutive days. A control group was included. After 10 days the rats were sacrificed and the brains were examined for morphological and histoenzymatic changes. Morphological changes included degenerative changes of neurocytes, accompanied with moderate proliferation of the oligodendroglia, and glial proliferation in the white matter. Furthermore, endothelial edema was observed in the small arterial and capillary walls. Histoenzymatic changes included decreased activities of ACP (acid phosphatase), ATPase (adenosinetriphosphatase), AChE (acetylcholine esterase), and BChE (Butyrylthiocholineesterase). The activities of TTPase (thiamine pyrophosphatase) and NSE (non-specific esterase) were increased. No details on quantitative aspects of enzymatic changes were given. No change was seen in the alkaline phosphatase. The authors indicated that observed morphological and histoenzymatic changes were unspecific, undistinctive and most likely reversible (Kozik et al. 1980). Examination of the neurosecretory function of the hypothalamus and the hypophysis in these animals showed an increased neurosecretion in cells of the supraoptic and paraventricular nucleus of the hypothalamus along with a declined neurosecretion in the hypophysis and an enhanced release of antidiuretic hormone in the neurohypophysis (Kozik et al. 1981). It is not clear whether these observations represent an adverse effect of zinc on the brain or whether they are secondary to changes somewhere else in the body.

Boric acid

- No relevant neurotoxicity data were identified for boric acid.

Human Health – Tier 2

Acute Mammalian (AT) Toxicity Score (H, M or L): L

Zinc borate was assigned a score of Low for acute mammalian toxicity based on oral and dermal LD₅₀ values greater than 2,000 mg/kg-bw. This score is based on data from 3 routes of exposure in two different species of animals.

- *Oral*: An LD₅₀ of >10,000 mg/kg was determined in rats (U.S. EPA 1991).
- *Oral*: An LD₅₀ of >5,000 mg/kg was determined in rats (Cerven 1992).
- *Oral*: An LD₅₀ of >10,000 mg/kg was determined in rats (Daniels et al. 1969).
- *Dermal*: An LD₅₀ of >10,000 mg/kg in both male and female albino rabbits (U.S. EPA 1991).
- *Inhalation*: An LD₅₀ of > 5 mg/L was determined (species unspecified) (EFRA 2006).

Corrosion/Irritation (Skin/ Eye) (Cr) Score (H, M or L): M

Zinc borate was assigned a score of Moderate for corrosion/irritation as both dermal and ocular irritation have been reported.

- *Dermal*: Contact with skin causes irritation (HSDB 2003).
- *Dermal*: The Primary Irritation Index of zinc borate in rabbits was found to be 0. Therefore, it is not considered to be an irritant or corrosive (U.S. EPA 1991).
- *Ocular*: Contact with eyes causes irritation (HSDB 2003).
- *Ocular*: Zinc borate produced only mild conjunctivitis in albino rabbits in the eye irritation test and is not considered to be an irritant or corrosive (U.S. Borax 1996).
- *Ocular*: Zinc borate was shown to be an eye irritant producing mild conjunctivitis in albino rabbits (U.S. EPA 1991).
- *Inhalation*: Inhalation of dust may irritate nose and throat (HSDB 2003).
- Zinc borates are not skin or eye irritants (no species or doses provided) (EFRA 2006).

Sensitization (Sn) Score (Skin and Respiratory) (H, M or L): L

Because sensitization data were sparse for zinc borate, the structurally similar zinc oxide and boric acid were used as surrogates. Zinc borate was assigned a score of Low for sensitization based on negative sensitization test results in surrogates.

Zinc borate

- *Dermal*: Zinc borate was negative in the guinea pig sensitization test (U.S. Borax 1996).

Zinc oxide

- The skin sensitization potential of zinc oxide (99.69% purity) was investigated in female Dunkin Hartley guinea pigs in two well-performed maximization tests, conducted according to Directive 96/54/EC B.6 and OECD guideline 406. Based on the results of a preliminary study, in the main studies experimental animals (10

in each test) were intradermally injected with a 20% concentration and epidermally exposed to a 50% concentration (i.e. the highest practically feasible concentration). Control animals (5 in each test) were similarly treated, but with vehicle (water) alone. Approximately 24 hours before the epidermal induction exposure, all animals were treated with 10% SDS. Two weeks after the epidermal application, all animals were challenged with a 50% test substance concentration and the vehicle. In the first study, in response to the 50% test substance concentration skin reactions of grade 1 were observed in 4/10 experimental animals 24 hours after the challenge (40% sensitization rate), while no skin reactions were evident in the controls. In contrast, in the second study no skin reactions were evident in the experimental animals (0% sensitization rate), while a skin reaction grade 1 was seen in one control animal. The skin reaction observed in one control animal is probably a sign of non-specific irritation (Van Huygevoort, 1999b1; 1999b2). In a third, well-performed maximization test, conducted according to the same guidelines and with the same experimental design, another analytical grade zinc oxide was tested (Zincweiß Pharma A; purity 99.9%). The only difference with the studies described above was the intradermal induction concentration, which was 2% as for Zincweiß Pharma A this was considered the highest concentration that could reproducibly be injected. In this test, no skin reactions were evident in both experimental and control animals, hence a 0% sensitization rate for Zincweiß Pharma A. White staining of the treated skin by the test substance was observed in some animals 24 and 48 hours after challenge (Van Huygevoort 1999i).

- In a human patch test performed with 100 selected leg-ulcer patients, 11/100 patients gave an allergic reaction with zinc ointment (60% ZnO and 40% sesame oil). However, 14/81 patients gave a positive response when treated with sesame oil alone (Malten and Kuiper 1974). This study does not give any indication for a skin sensitizing potential of zinc oxide in humans. Söderberg et al. (1990) studied the effect of zinc oxide on contact allergy to colophony. With 14 patients with earlier history of moderate patch test reactions to colophony a patch test with 10% ZnO (2.3 mg Zinc/cm²) with and without colophony was performed. No positive response was observed in the 14 patients when only a 10% solution of zinc oxide was used. The addition of zinc oxide to colophony decreased the allergic reaction induced by colophony.
- The data submitted fulfill the base-set requirements for skin sensitization testing. While some studies with guinea pigs produced conflicting results, the weight of evidence does not indicate that zinc oxide is a very potent sensitizing agent in animals, if any. In addition, the results of human patch tests do not indicate that zinc oxide acts as a sensitizing agent in humans, either. Zinc oxide does not have to be classified/labeled for skin sensitization. This is supported by the fact that zinc compounds, especially zinc oxide and zinc distearate, have been used for over decades in a variety of pharmaceutical and cosmetic products (some of them even dermatological preparations against skin irritation) without any such reported effects (ESIS 2008).

Boric acid

- Boric acid and sodium tetraborates are not skin sensitizers in either human and animal studies (Wnorowski 1994a,b,c; Bruze et al.1995).

Systemic/Organ (ST) Toxicity Score (includes organ effects and immunotoxicity) (H, M or L): M

Because systemic toxicity data were sparse for zinc borate, the structurally similar zinc oxide and boric acid were used as surrogates. Zinc borate was assigned a score of Moderate for systemic toxicity based on an oral LOAEL for systemic effects of 81.3 mg ZnO/kg bw.

Zinc borate

- In animal feeding studies, high levels of boric acid displays effects on fertility (rats, mice, dogs) and development (rats, mice, rabbits). High levels of zinc salts do cause adverse effects on fertility and development in animals, but at doses that perturb copper homeostasis resulting in other adverse effects. The doses administered were many times in excess of those which humans would be exposed and therefore the effects would not be seen in humans. A human epidemiology study on workers exposed to boric acid and sodium borates indicated no effect on fertility, while a study in pregnant women taking zinc supplements found no adverse effects. Zinc is an essential element for normal fetal development. Also, there is increasing evidence that boron is nutritionally important and may be essential for mammals (EFRA 2006).

Zinc oxide

- Four groups of ferrets (3-5/group) were given 0, 500, 1,500, or 3,000 mg zinc oxide/kg feed (equivalent to be 0, 81.3, 243.8 or 487.5 mg ZnO/kg bw, respectively. At the highest dose level (487.5 mg ZnO/kg bw) all animals (3) were killed in extremis within 13 days. Macroscopic examination showed pale mucous membranes, dark colored fluid in the stomach, blood in the intestines, orange colored liver and enlarged kidneys showing diffuse necrosis, hemorrhages in the intestine and a severe macrocytic hypochromic anaemia. Histology showed nephrosis and extramedullary hematopoiesis in the spleen. At the mid dose level of 243.8 mg ZnO/kg bw, the animals (4) were killed on day 7, 14 and 21 (1/2 in extremis) showing poor condition. Macroscopy showed pale livers with fatty infiltration and enlarged kidneys. Histology was comparable with the highest dose group. The hemogram showed macrocytic hypochromic anaemia, increased reticulocytes and leucocytosis. At the lowest dose level (81.3 mg ZnO/kg bw), the animals (3) were killed on day 48, 138 and 191, respectively. No clinical signs of toxicity or pathological changes were seen, apart from an extramedullary hematopoiesis in the spleen (Straube et al. 1980).
- Ellis et al. (1984) conducted a 14 day and a 49 day feeding study in 3 different breeds of sheep that were receiving feed containing 31 mg Zn²⁺/kg feed. The sheep received additional amounts of Zn²⁺ (from ZnO) at dose levels of 261 and 731 (14 day study), or 731 and 1,431 mg Zn²⁺/kg feed (49-day study). No effects were seen after 261 mg Zn²⁺/kg feed. In all other groups, pancreatic lesions were seen.
- Administration of 240 mg Zinc (as ZnO)/kg bw for 3 times/week during 4 weeks to 42 castrated sheep resulted in an increased incidence of pancreatic lesions (Smith and Embling 1993).

- Male Hartley guinea pigs were exposed to 0, 2.3, 5.9, or 12.1 mg/m³ of ZnO (as ultra fine particles with an average diameter of 0.05 µm) 3 hours a day for 1, 2, or 3 consecutive nose-only exposures. Three animals from each group were examined after each exposure period; they were sacrificed and lung tissues were microscopically examined, and the pulmonary lavage fluid was also examined. Exposure to 12.1 mg/m³ increased the number of nucleated cells in lavage fluid. Exposures to 5.9 and 12.1 mg ZnO/m³ were associated with increased protein, neutrophils, and activities beta glucuronidase, acid phosphatase, alkaline phosphatase, lactate dehydrogenase, and angiotensin-converting enzyme. The increases were dose dependent and were detectable after the second exposure and generally increased after the third exposure. Significant morphologic damage characterized by centriacinar inflammation in the lung was seen at 5.9 and 12.1 mg/m³. Minimal changes in neutrophils and activities of lactate dehydrogenase and alkaline phosphatase were seen in the pulmonary fluid at the lowest dose level of 2.3 mg/m³ after 3 exposures but no morphologic changes were observed at this dose level. Based on these results, 2.3 mg ZnO/ m³ is considered as a marginal LOAEL in this study (Conner et al. 1988).
- Male Hartley guinea pigs were exposed to 6 mg/m³ of ultra fine ZnO (average diameter of 0.05 µm) for 3 hours a day for 1 to 5 days by nose-only exposure. A control group was included. After each exposure, 3 animals were sacrificed and lung tissues were microscopically examined. After first, second and third exposure 3 additional animals were sacrificed and their pulmonary lavage fluid was examined. ZnO-exposure increased the total cell count, neutrophils, protein, and the enzyme activities of angiotensin converting enzymes, Acid phosphatase, alkaline phosphatase, and β -glucuronidase. Furthermore, a dose-related centriacinar inflammation was seen after second exposure (Conner et al. 1986).
- Male Hartley guinea pigs were exposed to 0, 2.7, or 7 mg ultra fine (0.05 µm in diameter) ZnO/m³ 3 hours a day for 5 days. Lung function measurements were performed every day after exposure in 5-8 animals. After the last exposure the animals were sacrificed. At the highest exposure level, a gradual decrease in total lung capacity (18%) and vital capacity (22%) was seen during the exposure period. At day 4, the carbon monoxide diffusing capacity dropped to below 30% of the control level. Wet-lung weights were increased with 29%, indicating the presence of edema. Exposures up to 2.7 mg ZnO/m³ did not alter any parameters measured (Lam et al. 1988).
- Male Hartley guinea pigs (73) were exposed (nose-only) 3 hours a day for 6 days to 5 mg ZnO/m³ (0.05 µm in diameter). A group of 53 animals served as control group. Lung function tests (in 38 animals) were performed and the respiratory tract of the animals was morphologically examined 1, 24, 48 and 72 hours after the last exposure. Furthermore epithelial permeability (5 animals at 1 and 24 hours) and DNA synthesis in epithelial cells (5 animals at 24, 48 and 72 hours) were determined. Vital and functional residual capacity, alveolar volume and carbon monoxide diffusing capacity were all decreased and did not return to normal values 72 hours after the last exposure. Lung weights were elevated due to inflammation, still present at 72 hours after last exposure (Lam et al. 1985).
- 240 Female Wistar rats (80/group) were exposed by inhalation to 15 mg ZnO/m³ for 1 hour, 4 hours or 8 hours a day for 5 days a week. 20 Animals/group were

sacrificed after 14, 28, 56, and 84 days and their lungs were examined for zinc content. It appeared that the highest daily exposure time resulted in the highest dry lung weights, independent of the duration of the experiment, while the zinc content remained almost constant. The absolute and relative (relative to dried weights of lung tissue) zinc content in the lungs was influenced by the duration of the experiment. After 84 days exposure the zinc content was significantly higher compared to 14 days exposure, independent of the duration of the daily exposure (Dinslage-Schlünz and Rosmanith 1976).

Boric acid

- A number of studies in which rats were fed boric acid or disodium tetraborate decahydrate in their diet or drinking water for periods of 70 - 90 days indicated that the main target organ for toxicity is the testis. As well as testicular atrophy, animals receiving doses of 88 mg B/kg bw/day for 90 days in their diet exhibited weight loss and, at higher doses, rapid respiration, inflamed eyes, swollen paws and desquamation of the skin on the paws (Weir and Fisher 1972; NTP 1987). The main effects observed were on the testis.

Ecotoxicity

Acute Aquatic (AA) Toxicity Score (H, M or L): H

Because acute aquatic toxicity data were limited for zinc borate, the structurally similar zinc oxide and boric acid were used as surrogates. Zinc borate was assigned a score of High for acute aquatic toxicity based on the risk phrases: R50-R53.

- Zinc borates are classified as Dangerous to the Environment, R50/R53, Very toxic to aquatic organisms/May cause long-term effects in the aquatic environment. Zinc borates are considered as ‘sparingly soluble salts’ based on their toxicity. However, both boron and zinc are essential micronutrients for the healthy growth of plants and other aquatic organisms (EFRA 2006).

Zinc oxide:

- Associated with risk phrases R50, R51, R52, and R53 (ESIS 2008).
- *Algae*: The two tests with the unicellular alga *Pseudokierchneriella subcapitata* (formerly known as *Selenastrum capricornutum*), in which two different grades of ZnO were tested (“Red seal grade”, purity 99.77%, and “EPM-grade”, purity 99.37%), resulted in 72-h ErC₅₀ values for dissolved zinc of 135 and 136 µg Zn/l, respectively, for endpoint specific growth rate. The 72-h NOErC values for dissolved zinc were 8 and 24 µg/l, respectively (Table 3.3.1: LISEC, 1997; Van Ginneken 1994a). These NOEC values suggest that Red seal-grade ZnO may be somewhat more toxic than EPM-grade ZnO, but because of some differences between the two tests (using either statistics to derive the NOEC or using the lowest test concentration that resulted in less than 10% effect as NOEC; and either measuring dissolved zinc in the stock solution or in the test waters) and the small difference between the NOEC values, a firm conclusion cannot be drawn. Although red-seal grade ZnO and EPM-grade ZnO both have a high purity, the former contains somewhat less impurities (soluble salts) and is somewhat less soluble than the latter (see also footnote 7 below Table 3.3.1). Based on these characteristics, a somewhat lower toxicity could be predicted for Red-seal ZnO

compared to EPM-grade ZnO, which seems to be not in agreement with the above test results. It is noted that similar growth inhibition tests with the same algal species have been conducted with either a soluble zinc compound or with zinc metal powder (see Table 3.3.2.a and Table 3.3.2.d, respectively, in Annex 3.3.2.A of the Risk Assessment Report on Zn metal). These tests and the above tests with ZnO, all using soft to very soft artificial test media, resulted in comparable NOEC values if expressed as dissolved zinc, i.e. NOEC values in the range of 5-50 µg/l, regardless whether a soluble or “insoluble” test compound was used.

- *Invertebrates*: A short-term *Daphnia magna* immobilization test with “EPM-grade” ZnO (purity 99.37%) resulted in a 48-h EC₅₀ for dissolved zinc of 1,760 µg/l and a 48-h NOEC for dissolved zinc of 280 µg/l (Table 3.3.1: Van Ginneken 1994b). It is noted that the 48-h NOEC of 280 µg/l from this short-term test is within a factor of 2 of a number of NOEC values (endpoints: survival, reproduction and/or growth) derived in longterm *D. magna* tests in which a soluble zinc salt was used as test compound (see Table 3.3.2.a in Annex 3.3.2.A of the Risk Assessment Report on Zinc metal).
- *Fish*: In a 96-h acute toxicity test with fish *Brachydanio rerio* (test compound “EPM-grade” ZnO, purity 99.37%), no effect was found for dispersed ZnO at 100 mg ZnO/l (limit test), thus the 96-h EC₅₀ is >100 mg ZnO/l, nominal concentration, equivalent to >80 mg Zn/l. The actual dissolved zinc concentration in this ZnO dispersion was 4,700 µg Zn/l (Table 3.3.1: Van Woensel 1994b).

Boric acid

- A summary of appropriate acute test results are detailed in Table 14. Eisler (2000) and Dyer (2001) have compiled numerous literature values. The most sensitive tests report that acute effects on fish are in the range of 10-20 mg-B/L although the quality of these studies was rated low (Reliability code 4). The lowest daphnid acute value is 133 mg-B/L. Algal and microbial inhibition studies (Table 15) suggest less toxicity: Selenastrum growth was not affected at 93 mg-B/L and activated sludge respiration showed minimal effects at 683 mg/L boric acid (119 mg-B/L).
- Other results showed substantially higher values (less toxicity) with fish acute values often exceeding 100 mg-B/L. Juveniles and fry appear to be the most sensitive fish life-stage (Hamilton 1995; Hamilton and Buhl 1990).
- Aquatic studies have been used to create species sensitivity distributions (SSD). SSD incorporate all available information into a summary statistic by calculating a designated percentile of the distribution, such as the 5th percentile. Such values indicate a concentration that is predicted to protect 95% of all species (included those not tested) (Cardwell et al. 1993). Dyer et al. (2001) calculated the Acute 5th percentile concentration for aquatic species. Using the procedure of Aldenberg and Slob (1993), the acute 5th percentile SSD concentration is 43 mg-B/L (246 mg-boric acid/L). Using a similar procedure of Stephan et al. (1985) produces a similar value, 46 mg-B/L (263 mg-boric acid/L).

Chronic Aquatic (CA) Toxicity Score (H, M or L): nd

Because chronic aquatic toxicity data were unavailable for zinc borate, the structurally similar zinc oxide and boric acid were used as surrogates. No relevant chronic aquatic toxicity data were identified for zinc borate, zinc oxide, or boric acid.

Zinc borate

- No relevant data were identified.

Zinc oxide

- No relevant chronic aquatic toxicity data were identified for zinc oxide.

Boric acid

- No relevant chronic aquatic toxicity data were identified for boric acid.

Environmental Fate

Persistence (P) Score (vH, H, M, or L): nd

Because persistence data were unavailable for zinc borate, the structurally similar zinc oxide and boric acid were used as surrogates. No relevant persistence data were identified for zinc borate, zinc oxide, or boric acid.

Zinc borate

- No relevant persistence data were identified for zinc borate.

Zinc oxide:

- No relevant persistence data were identified for zinc oxide.

Boric acid:

- No relevant persistence data were identified for boric acid.

Bioaccumulation (B) Score (vH, H, M, or L): L

Zinc borate was assigned a score of Low for bioaccumulation based on professional opinion.

- Zinc borate has a low bioaccumulation potential. Additionally, Firebrake ZB (zinc borate) will undergo hydrolysis in water to form boric acid and zinc hydroxide. Neither of these substances will biomagnify through the food chain (20 Mule Team 2002).

Physical Properties

Explosivity (Ex) Hazard Rating (H, M or L): L

Zinc borate was assigned a score of Low for explosivity as no basis for concern was identified.

- Not explosive (20 Mule Team 2000).

Flammability (F) Hazard Rating (H, M or L): L

Zinc borate was assigned a score of Low for flammability as no basis for concern was identified.

- NFPA rating of 0 assigned for flammability (i.e. zinc borate is not flammable) (Fisher Scientific 2007).

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