

# Green Screen Assessment for Red Phosphorus (CAS #7723-14-0)

## Green Screen Version 1.2 (CPA 2011a)

**Note: Draft Assessment -- Validation Has Not Been Performed on *this* Green Screen Assessment**

### Green Screen Assessment Prepared By:

Name: Kristen Schaefer, M.F.S.  
 Title: Associate Toxicologist  
 Organization: ToxServices LLC  
 Date: May 24, 2011

### Green Screen Assessment QC'd By:

Name: Margaret H. Whittaker, Ph.D., M.P.H., E.R.T., D.A.B.T  
 Title: Managing Director and Chief Toxicologist  
 Organization: ToxServices LLC  
 Date: June 2, 2011

### Also Called:

Amgard CPC, Amgard CPC 405, 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, 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 (ChemIDplus 2011).

### Chemical Structure(s):



### For Inorganic Chemicals and relevant particulate organics

#### Define Form & Physiochemical Properties

1. Particle size (e.g. silica of respirable size)- unknown
2. Structure (e.g. amorphous vs. crystalline)- Crystalline (O'Neil 2001)
3. Mobility (e.g. Water solubility, volatility)- 2.4 mg/L at 15°C; 4.1 mg/L at 25°C (ESIS 2000)
4. Bioavailability- Not bio-accessible (Pinfa 2010)

#### Identify Applications/Functional Uses: (e.g., Cleaning product, TV casing)

1. Flame retardant
2. Fertilizer
3. Pyrotechnics manufacturing

**Green Screen Rating<sup>1</sup>:** Red phosphorus was assigned a Benchmark Score of 2 based on High scores for systemic toxicity (ST), neurotoxicity (N), irritation/corrosion (IrS and IrE), and reactivity and flammability (Rx and F). *NOTE: Data gaps (dg) exist for Endocrine Activity (E) (not listed, but not tested), Carcinogenicity (C) and Respiratory Sensitization (SnR). In a worst-case scenario, if Red Phosphorus was assigned a High score for C and E it would be assigned a Benchmark Score of 1.*

Green Screen Hazard Ratings: Red Phosphorus																		
Group I Human					Group II Human							Ecotox		Fate		Physical		
C	M	R	D	E	AT	ST	N	SnS	SnR	IrS	IrE	AA	CA	P	B	Rx	F	
dg	L	L	L	dg	L	H	H	L	dg	H	H	M	M	M	vL	H	H	

\*Hazard levels (vH, H, M, L, vL) in *italics* reflect a lower level of confidence (See Guidance).

<sup>1</sup> For inorganic chemicals with low human and ecotoxicity across all hazard endpoints and low bioaccumulation potential, 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<sup>2</sup>

Functional Use	Life Cycle Stage	Transformation Pathway	Transformation Products	CAS #	On CPA Red List <sup>3</sup> ?	Green Screen Rating <sup>4</sup>
Insecticides and pesticides	Any	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 2011b).	1
Intermediate	End of Life	Combustion	Phosphorus acids	10294-56-1 and 13598-36-2	Not present on the Red List of Chemicals (CPA 2011b).	n/a
Intermediate	End of Life	Combustion	Polyphosphoric acids	8017-16-1	Not present on the Red List of Chemicals (CPA 2011b).	n/a
Drying agent, intermediate	End of Life	Decomposition	Phosphorus oxides	Multiple	Not present on the Red List of Chemicals (CPA 2011b).	n/a
Antioxidant	Any	Reaction with Water	Hypophosphrous acid	6303-21-5	Not present on the Red List of Chemicals (CPA 2011b).	n/a
Solvent	Any	Reaction with Water	Phosphoric acid	7664-38-2	Not present on the Red List of Chemicals (CPA 2011b).	n/a

### Introduction

Phosphorus exists in three main allotropic forms: white (sometimes called yellow phosphorus), black, and red (O'Neil 2001). Allotropes are different structural modifications of an element, where the atoms of the element are bonded together in a different manner.

<sup>2</sup> 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.

<sup>3</sup> Use the **most recent revision** of the CPA Red List spreadsheet (See Guidance).

<sup>4</sup> The way you conduct assessments for transformation products depends on the Benchmark Score of the parent chemical (See Guidance).

Red phosphorus is a stable transformation form of the element phosphorus (Leisewitz 2000). Toxicity data for red phosphorus produce conflicting conclusions; not all studies reviewed as part of the Green Screen state 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 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 are low, while inertial and micro-encapsulated red phosphorus do not pose a threat 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.

One significant hazard posed by the use of red phosphorus is that while being stored, a gradual release of toxic phosphine gas and other phosphoric acids may occur (Clariant Undated). The rate of decomposition into these more toxic substances depends directly on the amount of moisture available and temperature. To prevent this, manufactures must take special care to control the availability of moisture and oxygen and regulate temperature while storing red phosphorus. Additional solutions include adding stabilizers, using dust suppressants (oiling), and or coating the surface of the red phosphorus, a process called microencapsulation. By incorporating these processes into manufacturing, the stability of red phosphorus is improved, thus reducing possible health hazards.

The National Institute for Occupational Safety and Health (NIOSH) has assigned red phosphorus an exposure limit of 0.1 mg/m<sup>3</sup> (TWA) and an Immediately Dangerous to Life or Health value (IDLH) of 5 mg/m<sup>3</sup> (Avogadro 2000). OSHA assigned red phosphorus a Permissible Exposure Limit (PEL) of 0.1 mg/m<sup>3</sup> (Avogadro 2000).

## **Group I Human Health Effects (Group I Human)**

### **Carcinogenicity (C) Score (H, M or L): Data Gap**

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

### **Mutagenicity/Genotoxicity (M) Score (H, M or L): L**

Red phosphorus was assigned a score of Low for mutagenicity based on one animal study that suggests this substance is not mutagenic.

- Micronucleus analysis was performed on bone-marrow polychromatic and normachromatic red blood cells (RBC) and on circulating RBC of female rats exposed 8 times to red phosphorus/butyl rubber at 1.0 mg/L over a 2 week period for 2.25 hours. The author concluded the test substance was a weak clastogen. The results showed a significant clastogenic response in both bone marrow and RBC of rats that were exposed for 2 weeks, but that effect was not found after a 4-week exposure or after a 2-week recovery period. Effects after the 4-week exposure and 2-week recovery period would not be expected because micronuclei are removed from the circulation after 24 to 30 days. The fact that micronuclei are not observed after a 4-week exposure or a 2-week recovery period does not diminish the significance of observations at the end of the 2-week exposure period. These results are consistent with the conclusion that red phosphorus-butyl rubber is a weak clastogen. These results alone, however, do not allow a conclusion that red phosphorus-butyl rubber is mutagenic (Aranyi 1984).
- Red phosphorus was negative for mutagenicity in an OECD 471 Ames assay (Pinfa 2010).
- Red phosphorus was negative for chromosomal aberrations and gene mutations in Chinese hamster cells in an OECD 473 assay (Pinfa 2010).
- Because it is not bio-accessible, red phosphorus is not considered a potential genotoxicant (Pinfa 2010).

### **Reproductive Toxicity (R) Score (H, M, or L): L**

Red phosphorus was assigned a score of Low for reproductive toxicity based on one study in rats that showed it had no adverse effects on reproduction.

- There are no data to suggest that a single inhalation exposure to red phosphorus would cause reproductive toxicity (no other data provided) (U.S. EPA 2010).
- Because it is not bio-accessible, red phosphorus is not considered a potential reproductive toxicant (Pinfa 2010).
- Sprague-Dawley rats were exposed to a red phosphorus/butyl rubber mixture 5 days a week for 10 weeks at concentrations of 0.132 or 1.186 mg/L. No dominant lethal or single-generation reproductive effects were noted. Pregnant rats were also exposed in the same way for 5 days a week from gestation days 6 through 15. The fetuses were examined for skeletal and visceral anomalies. No dose-related increases were seen in any malformation or variations. In a single-generation study using the same exposure concentrations, offspring body weights were decreased on postnatal day (PND) 1 in the high-dose group, with a rebound in body weights in these pups at PNDs 14 and 21. Low-dose male and female offspring were heavier than controls at PNDs 4 to 21. No information was provided on body-weight gain or fertility in adults or on viability, survival, or lactation indices for the above studies. In a separate 12-week exposure study, nonpregnant Sprague-Dawley females in the high-dose group exhibited a significantly

lower weight gain after 4 weeks of exposure than females in the control or low-dose groups. No effects were reported on testicular toxicity in any of these studies. Because of the sparse data, a NOAEL cannot be established in terms of possible male and female reproductive toxicity (Weimer et al. 1980).

**Developmental Toxicity incl. developmental neurotoxicity (D) Score (H, M or L): L**

Red phosphorus was assigned a score of Low for developmental toxicity based on one study in rats that showed it had no adverse effects on reproduction.

- There are no data to suggest that a single inhalation exposure to red phosphorus would cause developmental toxicity (no other data provided) (U.S. EPA 2010).
- Because it is not bio-accessible, red phosphorus is not considered a potential developmental toxicant (Pinfa 2010).
- See the Weimer et al 1980 study.

**Endocrine Activity (A) Score (H, M or L): Data Gap**

- 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 2011b).
- Red phosphorus is not a suspected endocrine disruptor because it is not bio-accessible (Pinfa 2010).

**Group II Human Health Effects (Group II Human)**

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

Red phosphorus was assigned a score of Low for acute mammalian toxicity based on an oral LD<sub>50</sub> value greater than 2000 mg/kg and one inhalation LC<sub>50</sub> value between 2 and 10 mg/L, the cutoffs for high acute mammalian toxicity (CPA 2011a)

- *Oral*: An LD<sub>50</sub> of > 15,000 mg/kg-bw was determined for red phosphorus in rats (Clariant Undated, ESIS 2000, Pinfa 2010).
- *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 LC<sub>50</sub> (1 hour exposure) of 4.597 mg/L (red phosphorus/butyl rubber smoke) was determined in rats (Burton et al. 1982).
- *Inhalation*: An LC<sub>50</sub> (1 hour exposure to red phosphorus aerosol) of 1.217 mg/L (expressed as phosphorus) was determined in rats (Ballantyne 1998).
- *Inhalation*: An LC<sub>50</sub> (1 hour exposure to red phosphorus smoke) of 0.271 mg/L (expressed as phosphorus) was determined in mice (Ballantyne 1998).
- *Inhalation*: An LC<sub>50</sub> (1 hour exposure to red phosphorus smoke) of 1.689 mg/L (expressed as phosphorus) was determined in rabbits (Ballantyne 1998).
- *Inhalation*: An LC<sub>50</sub> (1 hour exposure to red phosphorus smoke) of 0.061 mg/L (expressed as phosphorus) was determined in guinea pigs (Ballantyne 1998).

**Systemic Toxicity/Organ Effects incl. immunotoxicity (ST) Score (vH, H, M or L): H**

Red phosphorus was assigned a score of High for systemic toxicity/organ effects based on animal studies that suggest it will produce specific target organ toxicity.

- 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).
- Male and female (5/sex/dose) Sprague-Dalwy rats were exposed in a static chamber to 1.128-1.882 mg/L of a red phosphorus/butyl rubber (360 g)/black powder (15 g) smoke mixture for 60-240 minutes and then observed for a 2 week period. Respiratory distress was observed in all animals. Other signs included transient hypoactivity, salivation, and conjunctivitis. There were no treatment related effects on body weight, hematologic or clinical chemistry indices, organ weights, or gross or microscopic lesions (Weimer et al. 1977).
- Beagle dogs (6/group; predominately males) were exposed in a static chamber to red phosphorus smoke at 1.212-1.882 mg/L for 30-240 minutes and observed for 2 weeks following exposure. A red phosphorus/butyl rubber (360 g) and black powder (15 g) mixture was ignited in the chambers and specific exposure concentrations maintained for specified durations. One dog in the 1.572 mg/L (180-min) exposure group died 4 days after exposure but the authors did not consider it treatment related. The remaining dogs survived the duration of the study. Signs of toxicity were primarily those of respiratory distress although there were no exposure-related lesions in the respiratory tract. There were no treatment-related changes in body weight, hematologic or clinical indices, organ weights, or gross or microscopic lesions. Conjunctivitis was observed in dogs exposed to the highest concentration but this was resolved by 3 days post exposure (Weimer et al. 1977).
- Male Porton-strain rats, Porton-strain mice, New Zealand white rabbits, and Dunkin-Hartley guinea pigs were exposure to smoke generated from pure unformulated red phosphorus for 1 hour. Smoke concentrations varied from species to species: rats and rabbits were exposed to 0.45, 0.87, 1.6, or 2.13 mg/L (expressed as phosphorus); mice were exposed to 0.111, 0.136, 0.22, 0.45, or 0.87 mg/L; guinea pigs were exposed to 0.036, 0.052, 0.111, or 0.45 mg/L. All animals that died showed similar histopathological findings in their respiratory tract. Major findings in rats, mice, and rabbits included laryngotracheal epithelial or mucosal necrosis with acute inflammatory cell infiltration, pulmonary congestion and edema, alveolar hemorrhages, alveolar wall polymorphonuclear cell infiltration, bronchiolitis, and macrophage aggregations in alveoli and bronchioles. These findings were more marked in the rabbits and less so in mice. Guinea pigs at the highest lethal concentrations showed no lesions in the larynx and trachea and only alveolar capillary congestion in the lungs (Ballantyne 1998).
- Female Porton Wistar-derived rats (5/group) were exposed to either a 95% red phosphorus and 5% butyl rubber mixture (3.2 mg/L) or a 97% red phosphorus and 3% butadiene styrene mixture (3.1 mg/L) for 30 minutes and then sacrificed at 24 hours or 14 days post exposure. One rat died during exposure to the red phosphorus/butyl rubber mixture and four rats died within the first 24 hours of exposure to the red

phosphorus/butadiene styrene mixture. Necropsy findings in the animals that died included laryngeal inflammation, blood in the tracheal lumen, severe pulmonary congestion, pulmonary edema, and hepatic congestion. With the exception of pulmonary edema, similar findings were seen in the surviving rats. All animals sacrificed on day 14 showed mild to moderate laryngeal inflammation and severe pulmonary congestion while those exposed to the red phosphorus/butadiene styrene mixture also exhibited mild alveolitis (Marrs 1984).

- 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).
- Male and female rats (10-20/group) were exposed to red phosphorus/butyl rubber combustion aerosol at concentrations of 2.00, 2.22, 2.62, 3.09, or 3.15 mg/L for 1 hour (1.2 hours at 3.15 mg/L) or 8.8 mg/L for 4 hours, and observed for 14 days. No animals died after exposure to 2.00 or 2.22 mg/L, 6% (1/18) died after exposure to 2.62 mg/L, and 20% (5/20) died after exposure to 3.09 and 20% (2/10) died in the 3.15 mg/L exposure group. Because no animals died after a single 4-hour exposure to 8.80 mg/L, the authors concluded that exposure concentration rather than duration was the determining factor for lethality. A marked decrease in body weight immediately after the exposure with gradual recovery starting about 9 days later was also noted. There did not appear to be gender-related variability in the inhalation toxicity of red phosphorus aerosol (Aranyi 1983).
- Male and female Sprague-Dawley rats were exposed to red phosphorus/butyl rubber aerosol mixture at concentrations ranging from 0.4 to 1.2 mg/L for 2.25 hours a day, 4 days a week, for 4 weeks. Male rats exposed to concentrations of 0.75 mg/L showed decreased white blood cell (WBC) counts. Female rats showed increased blood lymphocytes at the same concentration. In addition, significant increases in adenosine 5'-triphosphate (ATP) levels in macrophages lavaged from the lung, expressed as ATP/105 cells or ATP/total protein, were observed immediately after the last exposure at 0.75, 1.0, and 1.2 mg/L for male rats and at 0.40 and 0.75 mg/L for female rats (Aranyi 1983, 1984).

#### **Neurotoxicity (N) Score (vH, 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 2011b).
- In the experiment described above (Aranyi 1983, 1984) male rats showed increased motor activity at all concentrations and incomplete recovery after 2 weeks at some

concentrations. Females showed a trend toward increased activity but no evidence of such effect after the recovery period.

**Skin Sensitization (SnS) Score (H, M or L): L**

Red phosphorus was assigned a score of Low for skin sensitization because no basis for concern was identified.

- *Dermal*: Red phosphorus is not sensitizing to guinea pigs (ESIS 2000).

**Respiratory Sensitization (SnR) Score (H, M or L): Data Gap**

- No relevant data identified.

**Skin Irritation/Corrosivity (IrS) Score (vH, H, M or L): H**

Red phosphorus was assigned a score of High for skin irritation/corrosivity based on the potential for it to cause injury.

- *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).
- *Dermal*: Red phosphorus was slightly irritating to rabbits according to an FDA guideline 16 CFR 1500.41 91 26,141 assay (Pinfa 2010).

**Eye Irritation/Corrosivity (IrE) Score (vH, H, M or L): H**

Red phosphorus was assigned a score of High for eye irritation/corrosivity based on the potential for it to cause ocular injury.

- *Ocular*: May cause corneal injury (Avogadro 2000).
- *Ocular*: If contaminated with white phosphorus, contact can cause severe irritation and burns (J.T. Baker 2008).
- *Ocular*: Red phosphorus was not irritating to rabbits according to an FDA guideline 16 CFR 1500.42 91 26,142 assay (Pinfa 2010).
- *Ocular*: Conjunctivitis was reported in rats exposed at 1.813 mg/L for 189 minutes and in dogs exposed at 1.882 mg/L for 240 minutes. This resolved within 3 days after exposure ended (Weimer et al. 1977).

**Ecotoxicity (Ecotox)**

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

Red phosphorus was assigned a score of Moderate for acute aquatic toxicity based on the experimental L/EC<sub>50</sub> values that range from 10 to 100 mg/L, the criteria for moderate acute aquatic toxicity (CPA 2011a).

- An LC<sub>50</sub> of 2,609 mg/L was predicted in fish (96 hour) (U.S. EPA 2009).
- An LC<sub>50</sub> of 33 mg/L was determined in *Danio rerio* (freshwater fish, 96 hr) in an OECD guideline 203 study (Pinfa 2010)
- An LC<sub>50</sub> of 1,051 mg/L was predicted in daphnia (aquatic invertebrate, 48 hour) (U.S. EPA 2009).
- An LC<sub>50</sub> of 10.5 mg/L was determined in *Daphnia magna* (aquatic invertebrae, 48 hr) in an OECD guideline 202 study (Pinfa 2010).
- An EC<sub>50</sub> of 186 mg/L was predicted in green algae (aquatic plant, 96 hour) (U.S. EPA 2009).

- An EC<sub>50</sub> of 18.5 mg/L was determined in *Desmodesmus subspicatus* (algae, 72 hr) in an OECD guideline 201 study (Pinfa 2010)

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

Red phosphorus was assigned a score of Moderate for chronic aquatic toxicity based on it being assigned the following EU Risk Phrase: R52/53. Although the predicted chronic aquatic toxicity values indicate this substance to be of low concern, being included on this authoritative list will result in red phosphorus being assigned the default hazard score of moderate (CPA 2011a)

- Red phosphorus was assigned the following EU 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 predicted in fish (30 day) (U.S. EPA 2009).
- A ChV of 85 mg/L was predicted in daphnia (U.S. EPA 2009).
- A ChV of 48 mg/L was predicted in green algae (U.S. EPA 2009).

### **Environmental Fate (Fate)**

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

Red phosphorus was assigned a score of Moderate for persistence based on a half-life in soil that falls between 16 and 60 days, the range for moderate persistence (CPA 2011a).

- 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 2011).
- Because red phosphorus is an amorphous polymeric form of elemental phosphorus, it is not soluble in water and organic solvents. However, slow disproportionating and oxidizing reactions produce traces of toxic phosphine and phosphorus acids. These reaction products are the main cause of the toxic effects to organisms of red phosphorus. These reactions are promoted by high temperatures and moisture (Pinfa 2010).

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

Red phosphorus was assigned a score of Very Low for bioaccumulation based on a bioconcentration factor of less than 100, the cutoff for very low bioaccumulation (CPA 2011a).

- BCFBAF predicts a bioconcentration factor (BCF) of 0.9181 and a log K<sub>ow</sub> of -0.27 (U.S. EPA 2011).
- Because red phosphorus is an insoluble polymer, it is not expected to bioaccumulate (Pinfa 2010).

### **Physical Hazards (Physical)**

#### **Reactivity (Rx) Score (vH, H, M or L): H**

Red phosphorus was assigned a score of High for reactivity based on it being assigned the following EU 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) Score (vH, H, M or L): H**

Red phosphorus was assigned a score of High for flammability based on it being assigned the following EU Risk Phrase: R11.

- Red phosphorus was assigned the following Risk Phrase: R11- Highly flammable (Avogadro 2000, ChemCAS 2004, J.T. Baker 2008).

## References

Aranyi, C. 1983. Research and development on inhalation toxicologic evaluation of red phosphorus/butyl rubber combustion products. Phase II Report. U. S. Army Medical Research and Development Command, Fort Detrick, Frederick, MD. As cited in BEST 1997 and U.S. EPA 2010.

Aranyi, C. 1984. Research and development on inhalation toxicologic evaluation of red phosphorus/butyl rubber combustion products. Phase III Report. U. S. Army Medical Research and Development Command, Fort Detrick, Frederick, MD. As cited in BEST 1997 and U.S. EPA 2010.

Avogadro. 2000. MSDS for Phosphorus, Red. Available:  
<http://avogadro.chem.iastate.edu/MSDS/p-red.htm>

Ballantyne, B. 1998. Acute inhalation toxicity of red phosphorus smoke. *Tox Sub Mech*, 17:251-266.

Board of Environmental Studies and Toxicology (BEST). 1997. Toxicity of Military Smokes and Obscurants. Volume 1. National Academy Press, Washington DC.

Burton, F.G., M.L. Clark, R.A. Miller, and R.E. Schirmer. 1982. Generation and characterization (*sic*) of red phosphorus smoke aerosols for inhalation exposure of laboratory animals. *Am. Ind. Hyg. Assoc. J.* 43:767-772. As cited in U.S. EPA 2010.

ChemCAS. 2004. MSDS for Phosphorus Red Amorphous. Available:  
[http://www.chemcas.com/material/cas/archive/7723-14-0\\_v2.asp](http://www.chemcas.com/material/cas/archive/7723-14-0_v2.asp)

ChemIDPlus. 2010. Entry for phosphorus. United States National Library of Medicine. Available: <http://chem.sis.nlm.nih.gov/chemidplus/chemidheavy.jsp>

Clariant. Undated. Improvements in stability of red phosphorus. Available:  
[http://www.pa.clariant.com/C1256C70004EEA54/vwLookupDownloads/Red\\_Phosphorus\\_improved\\_stability.pdf/\\$FILE/Red\\_Phosphorus\\_improved\\_stability.pdf](http://www.pa.clariant.com/C1256C70004EEA54/vwLookupDownloads/Red_Phosphorus_improved_stability.pdf/$FILE/Red_Phosphorus_improved_stability.pdf)

Clean Production Action (CPA). 2011a. DRAFT- The Green Screen for Safer Chemical Version 1.2. Available: [http://www.cleanproduction.org/library/cpa-fact%20grscreen\\_Jan09\\_final.pdf](http://www.cleanproduction.org/library/cpa-fact%20grscreen_Jan09_final.pdf)

Clean Production Action (CPA). 2011b. Red List of Chemicals. Available:  
<http://www.cleanproduction.org/Greenscreen.php>

European Chemical Substances Information System (ESIS). 2000. IUCLID Dataset for phosphorus. European Commission Joint Research Centre. Available:  
<http://ecb.jrc.ec.europa.eu/iuclid-datasheet/7723140.pdf>

Grandjean, P. and P.J. Landrigan. 2006. Developmental neurotoxicity of industrial chemicals. *Lancet* 368: 2167-2178.

Hayes, W.J. and E.R. Laws (eds). 1991. Handbook of Pesticide Toxicology. Volume 2. Classes of Pesticides. New York, NY: Academic Press, Inc. As cited in HSDB.

Hazardous Substances Data Bank (HSDB). 2010. Entry for phosphorus. United States National Library of Medicine. Available: <http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?./temp/~qbxXdX:1>

J.T. Baker. 2008. MSDS for Phosphorus Amorphous. Available: <http://www.jtbaker.com/msds/englishhtml/p4017.htm>

Leisewitz, A, H. Kruse, and E. Schramm. 2000. Substituting environmentally relevant flame retardants: assessment fundamentals. Volume I: Results and summary overview. Environmental Research Plan of the German Federal Ministry for the Environment, Nature Conservation and Nuclear Safety. Research Report 204 08 542 (old) 297 44 542 (new).

Marrs, T.C. 1984. Histological changes produced by exposure of rabbits and rats to smokes produced from red phosphorus. Toxicol. Lett. 21:141-146. As cited in U.S. EPA 2010.

Marrs, T.C., H. Colgrave, J. Edginton, P. Rice, and N. Cross. 1989. The toxicity of a red phosphorus smoke after repeated inhalation. J. Haz. Mat. 22:269-282. As cited in HSDB.

Pinfa. 2010. Human Health and Environmental Fact Sheet: Red Phosphorus. Available: [http://www.pinfa.eu/uploads/Documents/Exolit\\_RP.pdf](http://www.pinfa.eu/uploads/Documents/Exolit_RP.pdf)

O'Neil, M.J., A. Smith, P.E. Heckelman (ed.). 2001. The Merck Index- An Encyclopedia of Chemicals, Drugs, and Biologicals. 13<sup>th</sup> Edition. Whitehouse Station, NJ: Merck and Co., Inc.

United States Environmental Protection Agency (U.S. EPA). 2009. ECOSAR v1.00a. Washington, DC, USA.

United States Environmental Protection Agency (U.S. EPA). 2011. Estimation Programs Interface (EPI) Suite™ Web, v4.00, Washington, DC, USA.

United States Environmental Protection Agency (U.S. EPA). 2010. Proposed acute exposure guideline levels (AEGs) for red phosphorus. Office of Pollution Pesticides and Toxins (OPPT). Available: [http://www.epa.gov/oppt/aegl/pubs/red\\_phosphorus\\_proposed\\_mar\\_2010\\_v1.pdf](http://www.epa.gov/oppt/aegl/pubs/red_phosphorus_proposed_mar_2010_v1.pdf)

Weimer, J.T, G. Affleck, J. Preston, J. Lucey, and J. Manthei. 1977. The acute effects of single exposures to United Kingdom red phosphorus screening smoke in rats, guinea pigs, rabbits, and dogs. Army Armament Research and Development Command, Chemical Systems Lab, Aberdeen Proving Ground MD. As cited in U.S. EPA 2010.

Weimer, J.T., G.E. Affleck, R.L. Farrand, F.K. Lee, and R.J. Pellerin. 1980. The acute and chronic effects of repeated exposure to United Kingdom red phosphorus screening smokes in rats, mice, guinea pigs, and rabbits. Tech. Rep. ARCSL-TR-79053. Chemical Systems Laboratory, U.S. Army Armament, Munitions and Chemical Command, Aberdeen Proving Ground, Edgewood, Md. As cited in BEST 1997.

## Appendix 1 Modeling Results

- **EPISuite Results for Red Phosphorus (CAS #7723-14-0)**

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-m<sup>3</sup>/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-m<sup>3</sup>/mole (2.48E+003 Pa-m<sup>3</sup>/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-m<sup>3</sup>/mole (1.682E+001 Pa-m<sup>3</sup>/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. (m<sup>3</sup>/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 cm<sup>3</sup>/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-m<sup>3</sup>/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 for Red Phosphorus (CAS #7723-14-0)**

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