File No: STD/1510

July 2014

NATIONAL INDUSTRIAL CHEMICALS NOTIFICATION AND ASSESSMENT SCHEME (NICNAS)

PUBLIC REPORT

Silicon phosphate ($Si_3(PO_4)_4$)

This Assessment has been compiled in accordance with the provisions of the *Industrial Chemicals (Notification and Assessment) Act 1989* (the Act) and Regulations. This legislation is an Act of the Commonwealth of Australia. The National Industrial Chemicals Notification and Assessment Scheme (NICNAS) is administered by the Department of Health, and conducts the risk assessment for public health and occupational health and safety. The assessment of environmental risk is conducted by the Department of the Environment.

For the purposes of subsection 78(1) of the Act, this Public Report may be inspected at our NICNAS office by appointment only at Level 7, 260 Elizabeth Street, Surry Hills NSW 2010.

This Public Report is also available for viewing and downloading from the NICNAS website or available on request, free of charge, by contacting NICNAS. For requests and enquiries please contact the NICNAS Administration Coordinator at:

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Director
NICNAS

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SUMMARY

The following details will be published in the NICNAS *Chemical Gazette:*

ASSESSMENT REFERENCE	APPLICANT(S)	CHEMICAL OR TRADE NAME	HAZARDOUS CHEMICAL	INTRODUCTION VOLUME	USE
STD/1510	Clariant (Australia) Pty Ltd	Silicon phosphate ($Si_3(PO_4)_4$)	Yes	≤ 200 tonne/s per annum	Component of catalysts for fuel production

CONCLUSIONS AND REGULATORY OBLIGATIONS

Hazard classification
Based on the available information, the notified chemical is recommended for hazard classification according to the *Globally Harmonised System for the Classification and Labelling of Chemicals (GHS),* as adopted for industrial chemicals in Australia. The recommended hazard classification is presented in the table below.

Hazard classification	*Hazard statement*
Eye damage (Category 1)	H318 – Causes serious eye damage

Based on the available information, the notified chemical is recommended for hazard classification according to the *Approved Criteria for Classifying Hazardous Substances* (NOHSC, 2004) with the following risk phrase:

R41: Risk of serious damage to eyes

Human health risk assessment
Provided that control measures are in place to limit worker exposure, the notified chemical is not considered to pose an unreasonable risk to the health of workers.

When used in the proposed manner, the notified chemical is not considered to pose an unreasonable risk to public health.

Environmental risk assessment

On the basis of the assessed use pattern, the notified chemical is not considered to pose an unreasonable risk to the environment.

Recommendations

REGULATORY CONTROLS

Hazard Classification and Labelling

- The notified chemical should be classified as follows:
  - Eye damage (Category 1): H318 - Causes serious eye damage

The above should be used for products/mixtures containing the notified chemical, if applicable, based on the concentration of the notified chemical present and the intended use/exposure scenario.

CONTROL MEASURES

Occupational Health and Safety

- A person conducting a business or undertaking at a workplace should implement the following engineering controls to minimise occupational exposure to the notified chemical:
  - Enclosed, automated systems, where possible
  - Ventilation system including local exhaust ventilation

- A person conducting a business or undertaking at a workplace should implement the following safe work practices to minimise occupational exposure during handling of the notified chemical:
  - Avoid contact with skin and eyes
  - Avoid inhalation

- A person conducting a business or undertaking at a workplace should ensure that the following personal protective equipment is used by workers to minimise occupational exposure to the notified chemical:
  - Goggles, gloves, respiratory protection, if appropriate

  Guidance in selection of personal protective equipment can be obtained from Australian, Australian/New Zealand or other approved standards.

- A copy of the (M)SDS should be easily accessible to employees.

- If products and mixtures containing the notified chemical are classified as hazardous to health in accordance with the *Globally Harmonised System for the Classification and Labelling of Chemicals (GHS)* as adopted for industrial chemicals in Australia, workplace practices and control procedures consistent with provisions of State and Territory hazardous substances legislation should be in operation.

Disposal

- The notified chemical should be disposed of to landfill in accordance with local regulations for recycling, re-use or recovery.

Emergency procedures

- Spills or accidental release of the notified chemical should be handled by physical containment, collection and subsequent safe disposal.

Regulatory Obligations

Secondary Notification
This risk assessment is based on the information available at the time of notification. The Director may call for the reassessment of the chemical under secondary notification provisions based on changes in certain circumstances. Under Section 64 of the *Industrial Chemicals (Notification and Assessment) Act (1989)* the notifier, as well as any other importer or manufacturer of the notified chemical, have post-assessment regulatory obligations to notify NICNAS when any of these circumstances change. These obligations apply even when the notified chemical is listed on the Australian Inventory of Chemical Substances (AICS).

Therefore, the Director of NICNAS must be notified in writing within 28 days by the notifier, other importer or manufacturer:

(1) Under Section 64(1) of the Act; if
  - the notified chemical is imported in powder form;

or

(2) Under Section 64(2) of the Act; if
  - the function or use of the chemical has changed from a component of catalysts for fuel production or is likely to change significantly;
  - the amount of chemical being introduced has increased, or is likely to increase, significantly;
  - the chemical has begun to be manufactured in Australia;
  - additional information has become available to the person as to an adverse effect of the chemical on occupational health and safety, public health, or the environment.

The Director will then decide whether a reassessment (i.e. a secondary notification and assessment) is required.

(Material) Safety Data Sheet

The (M)SDS of the products containing the notified chemical provided by the notifier were reviewed by NICNAS. The accuracy of the information on the (M)SDS remains the responsibility of the applicant.

ASSESSMENT DETAILS

1. APPLICANT AND NOTIFICATION DETAILS

APPLICANT(S)
Clariant (Australia) Pty Ltd (ABN: 30 069 435 552)
Brandon Office Park, Building 5, L2
530-540 Springvale Rd
GLEN WAVERLEY, VIC 3150

NOTIFICATION CATEGORY
Standard: Chemical other than polymer (more than 1 tonne per year).

EXEMPT INFORMATION (SECTION 75 OF THE ACT)
Data items and details claimed exempt from publication: degree of purity, import volume.

VARIATION OF DATA REQUIREMENTS (SECTION 24 OF THE ACT)
Variation to the schedule of data requirements is claimed as follows: spectral data, all physico-chemical endpoints (exception: water solubility), acute oral toxicity, acute inhalation toxicity, skin irritation toxicity, repeated dose toxicity, in vitro genotoxicity, bioaccumulation, fish toxicity, Daphnia toxicity, algal toxicity and inhibition of bacterial respiration.

PREVIOUS NOTIFICATION IN AUSTRALIA BY APPLICANT(S)
None

NOTIFICATION IN OTHER COUNTRIES
REACH registration (2013)

2. IDENTITY OF CHEMICAL

CHEMICAL NAME
Silicon phosphate ($Si_3(PO_4)_4$)

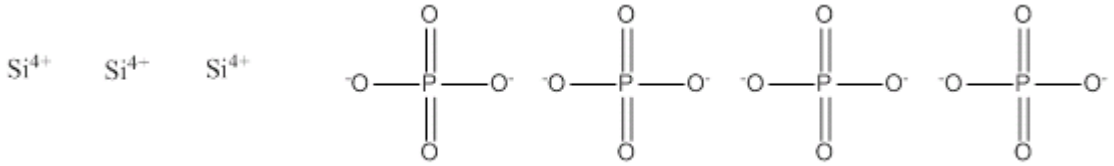
MARKETING NAME(S)
PolyMax 84x (products containing the notified chemical at ≤ 67% concentration)

OTHER NAME(S)
Silicon orthophosphate
Silicon phosphate

CAS NUMBER
12037-47-7

MOLECULAR FORMULA
$O_4P.Si$

STRUCTURAL FORMULA



MOLECULAR WEIGHT
464.142 Da

ANALYTICAL DATA
Crystallographic spectra were provided

3. COMPOSITION

DEGREE OF PURITY
> 80%

IDENTIFIED IMPURITIES/RESIDUAL MONOMERS

Chemical Name	2,4,6,7,8-Pentaoxa-3,5-diphospha-1-silatricyclo[3.1.1.11,3]octane, 3,5-dioxide (Silicon pyrophosphate)		
CAS No.	13827-38-8	*Weight %*	0–20%
*Hazardous Properties**	R41: Risk of serious damage to eyes R37: Irritating to respiratory system		

*Classification provided by notifier

ADDITIVES/ADJUVANTS
None

4. PHYSICAL AND CHEMICAL PROPERTIES

APPEARANCE AT 20 °C AND 101.3 kPa: Crystalline solid

Property	Value	Data Source/Justification
Melting Point/Freezing Point	> 1,000 °C	Chemical Safety Report, 2013
Density	2,360 kg/m^3 at 20 °C	Chemical Safety Report, 2013
Vapour Pressure	Not determined	Not applicable – the melting point of the chemical is above 300 °C
Water Solubility	1.085 g/L at 20 °C	Measured
Hydrolysis as a Function of pH	Not determined	Expected to hydrolyse following dissociation, mainly forming orthosilicic acid $H_4SiO_4/Si(OH)_4$
Partition Coefficient (n-octanol/water)	Not determined	As an inorganic compound, silicon orthophosphate is insoluble in n-octanol, making determination of a log Pow not feasible
Adsorption/Desorption	Not determined	Expected to combine indistinguishably with the soil or sediment due to its similarity with inorganic soil/sediment matter
Dissociation Constant	Not determined	Expected to dissociate readily, as an inorganic salt, into silicon and phosphate ions after introduction into the aquatic environment (pH 4 – 9)
Particle Size	Manufactured product 1: d50 = 11.695 mm* Manufactured product 2: d50 = 11.492 mm*	Granulometry testing of the two catalyst products containing the notified chemical (Chemical Safety Report, 2013)

Flash Point	Not determined	Not applicable. The chemical is a high melting point inorganic solid
Flammability	Not spontaneously flammable. No pyrophoricity. Does not emit flammable gases in contact with water.	(M)SDS
Autoignition Temperature	No self-ignition	Estimated, based on Melting Point data
Explosive Properties	Predicted negative	Does not contain explosophores
Oxidising Properties	Predicted negative	Does not contain oxidising functionality

* d50 is the median of the particle size distribution.

DISCUSSION OF PROPERTIES
For full details of tests on physical and chemical properties not discussed below, refer to Appendix A.

The notified chemical is an inorganic salt, which easily dissociates into silicon and phosphate ions after introduction into the aquatic environment (relevant pH values range from 4 – 9). The tetravalent silicon ion and the phosphate ion will then react with the media to form different silicon and phosphate species depending on the pH and redox potential of the media (Clariant, 2012a).

The dissociated silicon ion hydrolyses in water and exists predominantly as orthosilicic acid $H_4SiO_4/Si(OH)_4$, which is also the main species when silicon dioxide is dissolved in water. The dissociation constants of orthosilicic acid are high (pKa 9.9, 11.8, 12 & 12 at 30 °C, Lide & Frederikse 1995). The amount of soluble silicate rapidly decreases when the pH is lowered to 9 from strongly basic conditions. Because of this, at environmental pH values of 6.5 – 8.5 large amounts of the soluble silicon species might be gradually removed from the aqueous solution (OECD SIDS, 2004).

In the normal aquatic environment (pH 4 - 9), $H_2PO_4^-$ and HPO_4^{2-} are prevalent and are found in equilibrium. H_3PO_4 is expected to have pKa values of 2.15, 7.20, and 12.38 (Aylward and Findly, 1998).

Reactivity
The notified chemical is expected to be stable under normal conditions of use. It is not explosive or combustible and does not contribute to the spreading of active fires. However, when the notified chemical is exposed to an active fire, a haze containing phosphoric acid and oxides of phosphorus POx can form from its combustion and produce hazardous effects.

Physical hazard classification
Based on the submitted physico-chemical data depicted in the above table, the notified chemical is not recommended for hazard classification according to the *Globally Harmonised System for the Classification and Labelling of Chemicals (GHS),* as adopted for industrial chemicals in Australia.

5. INTRODUCTION AND USE INFORMATION

MODE OF INTRODUCTION OF NOTIFIED CHEMICAL (100%) OVER NEXT 5 YEARS
The notified chemical will be imported into Australia as a major component of finished catalyst products PolyMax 84x, containing the notified chemical at ≤ 67% concentration.

MAXIMUM INTRODUCTION VOLUME OF NOTIFIED CHEMICAL (100%) OVER NEXT 5 YEARS

Year	*1*	*2*	*3*	*4*	*5*
Tonnes	< 200	< 200	< 200	< 200	< 200

PORT OF ENTRY
Melbourne and Perth

IDENTITY OF MANUFACTURER/RECIPIENTS
Clariant (Australia) Pty Ltd

TRANSPORTATION AND PACKAGING
The notified chemical, as a component of the catalyst product PolyMax 84x, will be imported in the form of pelletised cylindrical extrusions, enclosed in 180 kg sealed polyethylene bags contained in steel 200 L drums and will be transported via road from the port of entry to commercial outlets for retail sale. In Perth, the imported products will usually be transported directly from the wharves to commercial customers. In Melbourne, the

imported products will undergo interim storage in the notifier's warehouse prior to distribution to commercial customers.

USE
The imported product containing the notified chemical (at ≤ 67% concentration) will be used exclusively in the petroleum refining industry. The notified chemical will be imported as a component of catalyst preparations and used in olefin oligomerisation to produce fuels and higher olefins.

OPERATION DESCRIPTION
Store handlers will move the drums containing the product PolyMax 84x catalysts (containing the notified chemical) from the delivery or storage position to the reactor by forklifts vehicles, crane and other suitable transport devices.

The reactors are fixed bed catalytic reactors of 10 m^3 to 80 m^3 capacity (depending on plant design). The reactor will be loaded with PolyMax 84x catalyst once every three to six months. Loading of the catalyst into the reactor will be accomplished at a typical rate of 6 tonnes per hour. Unloading the catalyst from the reactor will be accomplished at a typical rate of 4 tonnes per hour, but can vary depending on the consistency of the spent catalysts. Contract loading and unloading crews will typically work 10 hours per day. Typically the loading and unloading of the catalyst into the reactor will be subcontracted to specialised service companies.

The catalyst will not normally be weighed on site as the delivered drums will be loaded with a fixed weight. Loading will be via a vacuum transfer of the pelletised catalyst containing the notified chemical into a loading hopper. The catalyst will fall by gravity into the fixed bed catalytic reactor. In case personnel have to enter the reactor, special personal protection will be applied according to safety standards.

Normally, no residues will be left in the drum inner liner bag. Used packaging will normally be disposed to approved landfill or re-used for storing the spent catalyst. Laboratory technicians will perform physical and/or chemical quality control tests on the catalyst samples taken during loading operations.

After the catalyst is loaded, the reactor will be closed and the feed (olefin hydrocarbon) passed over the catalyst according to a set time, temperature and pressure. The process will be continuous (24 hours for 7 days). During this time, the reactor will be completely sealed. Operators will not be exposed to the catalyst nor to feed or product streams.

The typical life time of the catalyst is three to six months and it cannot be regenerated. The spent catalyst will be unloaded from the reactor by specialised service companies. Unloading will be done by either gravity, water jet or jack hammer (depending on the consistency of the spent catalyst). It may take hours to one week (depending on the size of the reactor and the consistency of the spent catalyst). The spent catalyst will then be stored in drums with an inner liner and disposed of through a licensed waste contractor to an approved landfill site.

6. HUMAN HEALTH IMPLICATIONS

6.1. Exposure Assessment

6.1.1. Occupational Exposure

CATEGORY OF WORKERS

Category of Worker	*Exposure Duration (hours/day)*	*Exposure Frequency (days/year)*
Store personnel (Clariant)	2	4
Store personnel (end-user company)	2	4
Laboratory technicians	2	4
Contract loaders/unloaders	10	20

EXPOSURE DETAILS
The notified chemical is a component of the catalyst product PolyMax 84x acting in olefin oligomerisation processes. Such petroleum refinement occurs in an enclosed industrial process. The notifier states that workers are not expected to be directly exposed to the notified chemical during the function of the reactor.

Transport and storage workers are unlikely to be exposed to the notified chemical except in the event of an accident. The notifier states that exposure to workers (e.g. during transfer processes, maintenance of associated equipment or inadvertent spillage or release), is expected to be minimised through the use of mechanical ventilation and/or enclosed systems and through the use of personal protective equipment (PPE) such as coveralls, safety glasses and impervious gloves. Exposure to the notified chemical via the oral route is unlikely considering the proposed use pattern. Inhalation exposure is unlikely given the estimated low vapour pressure of the notified chemical and the granular nature of the catalyst products containing the notified chemical. However, the notifier states that some dust may be generated during loading operations and workers with potential exposure to the notified chemical via the inhalation route are expected to wear respiratory protection.

6.1.2. Public Exposure

The notified chemical will be used as a component of catalyst preparations exclusively in the petroleum refining industry and is not intended for use by the public. Public exposure is expected to occur only in the event of a transport accident.

6.2. Human Health Effects Assessment

The results from toxicological investigations conducted on the notified chemical are summarised in the following table. For full details of the studies, refer to Appendix B.

Endpoint	*Result and Assessment Conclusion*
Rat, acute dermal toxicity	LD50 > 2,000 mg/kg bw; low toxicity
Eye irritation (in vitro)	severely irritating
Mouse, skin sensitisation – Local lymph node assay	no evidence of sensitisation
Mutagenicity – bacterial reverse mutation	non mutagenic

Additional information (briefly discussed in text below) was provided for the chemicals, silicon dioxide (CAS no. 7631-86-9) and phosphoric acid, potassium salt (1:2) (CAS no. 7758-11-4) (Chemical Safety Report, 2013, REACH, 2013). As noted above, the notified chemical easily dissociates into silicon and phosphate ions and collectively, these substances yield the same ions as the target substance (either ionic silicon or ionic orthophosphate) when dissolved in water (Clariant, 2012a).

Toxicokinetics, metabolism and distribution.

There are no studies available on the notified chemical regarding toxicokinetic properties. As noted above, the notified chemical is an inorganic salt, which easily dissociates into silicon and phosphate ions once introduced into an aqueous environment, e.g. if ingested. The notifier has indicated that based on the relatively low molecular weight (< 500 Da) and high water solubility (1.085 g/L at 20 ºC) of the notified chemical, and taking the properties of silicon dioxide and phosphorus compounds into consideration, that absorption and wide distribution throughout the body is possible and that the notified chemical is not subject to any metabolism (Chemical Safety Report, 2013).

Acute toxicity.

The notified chemical was of low acute dermal toxicity. Grade 1 erythema was noted in one of the five female test animals on day 3 and 4 of the observation period and scratches and eschar were observed in all male and female animals up until day 9. No oedema was observed in any animals during the test period. All clinical signs had resolved by day 10 of the study period. The study authors acknowledged the signs of dermal irritation but concluded that the notified chemical showed no signs of acute dermal toxicity.

No acute oral or inhalation toxicity data are available for the notified chemical.

Irritation and sensitisation.

A skin irritation study was not available for the notified chemical. However, significant/non-reversible irritant effects were not observed in an acute dermal toxicity study in rats (up to 2,000 mg/kg bw applied; 24 hour exposure period; see above for discussion of the observed responses).

The notified chemical was severely irritating in a bovine corneal opacity and permeability test (BCOP), with an in vitro irritancy score (IVIS) of 93.13 calculated.

In a local lymph node assay (LLNA) performed with the notified chemical, no sensitising effects were observed.

Repeated dose toxicity.
No subchronic studies are available for the notified chemical. The following repeated dose toxicity study summaries were provided for the chemicals, silicon dioxide and phosphoric acid, potassium salt (1:2) (Chemical Safety Report, 2013).

A 90-day repeated dose toxicity study was conducted with silicon dioxide (SiO_2), where rats were exposed to the chemical at doses ranging from 300 to 4,500 mg/kg bw/day in the feed. No signs of toxicity were noted based on clinical, haematological, urinary and histopathological examinations. Based on the lack of any observed adverse effects seen in any of the dosed groups, the NOAEL was established for silicon dioxide at ≥ 4,000–4,500 mg/kg bw/day (the highest dose tested).

Several study summaries were provided for the chemical, phosphoric acid, potassium salt (1:2). For example, a 22 week repeated dose toxicity (feed) study in dogs was conducted and a LOAEL of 1,000 – 2,000 mg/kg bw/day and NOAEL of < 800 mg/kg bw/day were determined, reportedly based on the nephrocalcinosis seen during kidney histopathology in the animals treated at higher doses. This effect is reportedly commonly observed after uptake of high doses of phosphate compounds (Clariant, 2012a).

Mutagenicity/Genotoxicity.
In a bacterial reverse mutation assay, the notified chemical did not cause gene mutations by base pair changes or frameshifts in the genome of the tester strains used, both in the presence or absence of metabolic activation. The notified chemical was therefore considered to be non-mutagenic.

In addition, summaries of in vitro genotoxicity studies conducted on the chemical, silicon dioxide, were also provided. A mammalian chromosome aberration test and a gene mutation test on Chinese hamster ovary cells rendered negative results.

Health hazard classification
Based on the available information, the notified chemical is recommended for hazard classification according to the *Globally Harmonised System for the Classification and Labelling of Chemicals (GHS),* as adopted for industrial chemicals in Australia. The recommended hazard classification is presented in the following table.

Hazard classification	*Hazard statement*
Eye damage (Category 1)	H318 – Causes serious eye damage

Based on the available information, the notified chemical is recommended for hazard classification according to the *Approved Criteria for Classifying Hazardous Substances* (NOHSC, 2004), with the following risk phrase(s):
R41: Risk of serious damage to eyes

6.3. Human Health Risk Characterisation

6.3.1. Occupational Health and Safety
Workers will be exposed to the notified chemical as a component of catalyst preparations at a concentrations ≤ 67%. The notified chemical is considered to be severely irritating to the eyes and at the proposed usage concentration, the risk of eye irritation effects is a concern. However the notified chemical is proposed to be used strictly in conjunction with adequate PPE, specifically eye protection, reducing the potential for exposure.

While there is no data on the acute oral toxicity of the notified chemical, ingestion is unlikely under the occupational settings described. While dermal absorption of the notified chemical is possible, it was shown to be of low acute toxicity via the dermal route. In addition, PPE (including gloves and appropriate clothing) is expected to be worn by workers to minimise the potential for dermal exposure. While the particle size of the catalyst products containing the notified chemical, in combination with the proposed control measures (enclosed operations, exhaust ventilation, automated operations) suggest limited potential for inhalation exposure to the notified chemical, given the potential for dust generation during loading operations and that information on the toxicity of the notified chemical via the inhalation route is unavailable, PPE (respiratory protection), should be utilised to further lower the risk of exposure, if appropriate.

Provided that control measures are in place to minimise worker exposure to the notified chemical, the risk to the health of workers from use of the notified chemical is not considered to be unreasonable.

6.3.2. Public Health

The notified chemical is intended for exclusive use in industrial settings by trained workers. The public may only be exposed to the notified chemical in the unlikely event of an accident during transport. Therefore, when used in the proposed manner, the risk to public health from the notified chemical is not considered to be unreasonable.

7. ENVIRONMENTAL IMPLICATIONS

7.1. Environmental Exposure & Fate Assessment

7.1.1. Environmental Exposure

RELEASE OF CHEMICAL AT SITE
The notified chemical will be imported as a component of a catalyst product for direct use in olefin oligomerisation in the petroleum refining industry. Environmental release of the notified chemical is unlikely during importation, storage and transportation, with spillage during a transport accident the most likely reason for environmental release. When used as a catalyst, the product containing the notified chemical will be transferred from drum to the reactor vessel, followed by reactants. Incidental spills during loading/unloading of the notified chemical into reactor vessels are estimated to be less than 0.6% of the import volume, and will be properly collected and stored into drums for disposal to approved landfill.

RELEASE OF CHEMICAL FROM USE
The use of the imported notified chemical will be confined to a small number of petroleum refinery sites. Its function as a fixed bed reactor catalyst means that there will be no notified chemical present/remaining in the higher chain hydrocarbon (end product). All of the notified chemical will become inactive (spent) at the end of its process cycle. After use, the notified chemical will be removed and stored in drums with inner polyethylene (PE) liners for disposal by a licensed contractor to approved landfill sites.

RELEASE OF CHEMICAL FROM DISPOSAL
The need for disposal of the unused waste notified chemical would be limited and would only occur if spillage occurred. Due to the pelletised consistency of the notified chemical, only a negligible amount (50 - 100 grams) of residual chemical may remain within used packaging (drum liners) which are expected to be disposed by a licensed contractor to approved landfill. All the spent catalyst containing the notified chemical is expected to be collected for proper disposal which is most likely to an approved landfill.

7.1.2. Environmental Fate
As an inorganic substance, the notified chemical is not amenable to photo- or biodegradation. For the notified chemical, as well as its products of dissociation, bioaccumulation is not expected.

Most of the notified chemical is expected to be released to landfill as collected used chemical or from minor spills. In landfill, it is expected to combine with the soil or sediment, due to its similarity with inorganic soil/sediment matter and will be subjected to natural processes under environmental conditions (cation exchange, dissolution, sedimentation).

Of the elemental composition of the earth's crust, silicon is the second most abundant element after oxygen, i.e. 28% (Salminen, 2012). Silicon oxides are the most abundant compounds in the earth's crust mass (> 60%; Salminen, 2012). By weathering of soil, rocks and sediments, etc., silica is released into surface and ground waters from where it may be removed by precipitation and sedimentation. It can also be taken up by living organisms, especially diatoms as normal process mainly related to structural function. Compounds of silicon, oxygen and phosphorus are ubiquitous in the environment. The notified chemical is expected to remain present in inorganic matter, like minerals and soils.

7.1.3. Predicted Environmental Concentration (PEC)
The Predicted Environmental Concentration (PEC) has not been calculated since no significant level of release of the notified chemical to the aquatic environment is expected based on the proposed use pattern.

7.2. Environmental Effects Assessment
No ecotoxicity data were submitted for the notified chemical itself. Below are judgments for the toxicity of the notified chemical based on inorganic chemicals that are similar in structure (REACH, 2013; Clariant, 2012b).

Endpoint	*Result*	*Assessment Conclusion*
Fish Toxicity	96 h LC50 > 100 mg/L	Not harmful

Daphnia Toxicity	48 h EC50 > 100 mg/L	Not harmful
Algal Toxicity	72 h EC50 > 100 mg/L	Not harmful
Inhibition of Bacterial Respiration	3 h EC50 > 1000 mg/L	Not harmful

The notified chemical is readily soluble in water, dissociating into silicon and phosphate ions. Consequently, the chemical assessment is based on the products of dissociation. All aquatic toxicity end points indicate that the notified chemical is not harmful to aquatic organisms.

The notified chemical is not harmful to aquatic organisms based on the above endpoints. Therefore, it is not formally classified for acute and long term hazard to aquatic life under the Globally Harmonised System for the Classification and Labelling of Chemicals (GHS; United Nations, 2009).

Fish Toxicity - analogue study observations.
The substances which were chosen for the read across approach yield the same ions as the target substance (either ionic silicon or ionic orthophosphate) when dissolved in water. Data from phosphoric acid, potassium salt (2:3), dihydrate (CAS No. 6922-99-4) were used to cover the short-term toxicity to fish of the phosphate moiety of the substance. Data from silicon dioxide (CAS No. 17631-86-9) were used to cover the silicon moiety of the substance.

Phosphoric acid, potassium salt (2:3), dehydrate (CAS No. 6922-99-4) was tested in a 96 h limit test according to OECD 203 following good laboratory practice (GLP) with rainbow trout (*Oncorhynchus mykiss*) as the test organism. At a nominal test concentration of 100 mg/L, no mortality occurred in the control and test groups. Analysis of the test preparations at 0, 24 and 96 h showed measured test concentrations to range from 109% to 118% of nominal. Therefore, an LC50 (96h) > 100 mg/L (nominal) was assumed.

Silicon dioxide (CAS No. 7631-86-9) was tested in a 96 h GLP-guideline study according to OECD 203 without analytical verification of the test substance concentrations. Zebra fish (*Brachydanio rerio*) were exposed to test suspensions at nominal concentrations of 1,000 and 10,000 mg/L that were used after settling. As no mortality or adverse effects occurred in the control and test groups, an LL0 (96 h) = 10,000 mg/L was assumed.

Therefore, based on the read across approach an LC50 (96 h) > 100 mg/L can be assumed for silicon orthophosphate.

Daphnia Toxicity - analogue study observations.
The substances which were chosen for the read across approach yield the same ions as the target substance (either ionic silicon or ionic orthophosphate) when dissolved in water. Data from phosphoric acid, potassium salt (2:3), dihydrate (CAS No. 6922-99-4) are used to cover the short-term toxicity to aquatic invertebrates of the phosphate moiety of the substance. Data from silicon dioxide (CAS No. 7631-86-9) are used to cover the silicon moiety of the substance.

Phosphoric acid, potassium salt (2:3), dehydrate (CAS No. 6922-99-4), was tested in a 48 h limit test according to OECD 202 under GLP conditions, including analytical verification of the test substance concentrations. At a nominal test concentration of 100 mg/L, no mortality occurred in the control and test groups. Therefore, an EC50 (48h) > 100 mg/L was assumed.

Silicon dioxide (CAS No. 7631-86-9) was tested in a 24 h GLP-study without analytical verification of the test substance concentrations. Test suspensions at nominal concentrations of 1,000 and 10,000 mg/L were used after settling. As no immobilisation or adverse effects occurred in the control and test groups, an EL50 (24h) > 10,000 mg/L (nominal) was assumed.

Therefore, based on the read across approach an EC50 (48 h) > 100 mg/L can be assumed for silicon orthophosphate.

Algal Toxicity - analogue study observations.
The substances which were chosen for the analogue read across approach yield the same ions as the target substance (either ionic silicon or ionic orthophosphate) when dissolved in water. Data from phosphoric acid, potassium salt (2:3), dihydrate (CAS No. 6922-99-4) are used to cover the toxicity to algae of the phosphate moiety of the substance. Data from sodium aluminum silicate (CAS No. 1344-00-9) are used to cover the silicon moiety of the substance.

Algal toxicity of phosphoric acid, potassium salt (2:3), dehydrate (CAS No. 6922-99-4) was investigated in a 72 h limit test according to OECD 201 and GLP, including analytical verification of the test substance concentrations. At a nominal test concentration of 100 mg/L, no inhibition of growth rate and no abnormalities of the cells could be observed. Analysis of the test preparations at 0 and 72 h showed measured test concentrations to range from 107% to 113% of nominal values. Therefore, an E_rC50 (72h) > 100 mg/L and a $NOE_rC \geq 100$ mg/L based on nominal concentrations were assumed.

Sodium aluminum silicate (CAS No. 1344-00-9) was tested in a 72 h study according to OECD 201 and GLP, without analytical verification of the test substance concentrations. Algae were exposed to filtered test solutions at nominal concentrations of 96, 1008 and 10,000 mg/L. As no inhibition of algal growth and no abnormalities occurred, an E_rL50 (72h) > 10,000 mg/L (nominal) was stated.

Therefore, based on the read across approach an E_rC50 (72h) > 100 mg/L and NOEC (72h) ≥ 100 mg/L can be assumed for silicon orthophosphate.

Inhibition of Bacterial Respiration - analogue study observations.

The substances which were chosen for the read across approach yield the same ions as the target substance when dissolved in water. Data from dipotassium hydrogenorthophosphate (CAS: 7758-11-4) are used to cover the toxicity to bacteria of the phosphate moiety of the substance.

Dipotassium hydrogen orthophosphate (CAS: 7758-11-4) was tested in a GLP study according to OECD guideline 209 using predominantly domestic activated sludge as inoculum. After a contact time of 3 h, no inhibition of microbial respiration occurred up to 1000 mg/L which was the highest test concentration. Therefore, an EC50 (3h) > 1000 mg/L and a NOEC ≥ 1000 mg/L was stated.

No data are available for the silicon moiety. The absence of toxicity for activated sludge in sewage treatment plants can be safely assumed based on the absence of aquatic toxicity of synthetic amorphous silica and silicates in general. The assumption is also based on the fact that silicon dioxide is known to be utilised by aquatic organisms such as diatoms, radiolarians and silicoflagellates and thus can be considered to be a part of the environment. This assumption is supported by public assessments for synthetic amorphous silica and silicates (OECD, 2004).

Therefore, the effects on aquatic micro-organisms for silicon orthophosphate can be expected as EC50 (3h) > 1000 mg/L.

7.2.1. Predicted No-Effect Concentration

The PNEC was not calculated since no effects for the notified chemical are expected based on the estimated low ecotoxicity of the dissociation products, and no significant release of the notified chemical to the aquatic environment is expected.

7.3. Environmental Risk Assessment

The Risk Quotient (RQ = PEC/PNEC) has not been calculated since the PEC or PNEC were not calculated.
The notified chemical is not considered to pose an unreasonable risk to the environment based on the assessed use pattern and the expected low toxicity to aquatic organisms.

APPENDIX A: PHYSICAL AND CHEMICAL PROPERTIES

Water Solubility 1.085 g/L at 20 °C

Method	OECD TG 105 Water Solubility
Remarks	Flask Method. Mixtures of the notified chemical in water at 6.7 g/L were prepared and stirred for up to 192 hours at 20 °C until equilibrated concentrations were achieved. The concentrations of the notified chemical were analysed using inductively coupled plasma (ICP). The average of the measured solubilities was 1.085 g/L.
Test Facility	Clariant (2012b)

APPENDIX B: TOXICOLOGICAL INVESTIGATIONS

B.1. Acute toxicity – dermal

TEST SUBSTANCE	Notified chemical
METHOD	OECD TG 402 Acute Dermal Toxicity – Limit Test. EC Council Regulation No 440/2008 B.3 Acute Toxicity (Dermal) – Limit Test.
Species/Strain	Rat/WISTAR Crl: WI(Han)
Vehicle	Moistening with *aqua ad injectionem*
Type of dressing	Semi-Occlusive
Remarks - Method	GLP Certificate No significant protocol deviations.

RESULTS

Group	*Number and Sex of Animals*	*Dose mg/kg bw*	*Mortality*
1	5M	2,000	0/5
2	5F	2,000	0/5

LD50	> 2,000 mg/kg bw
Signs of Toxicity - Local	One female animal exhibited grade 1 erythema on day 3 and 4. No other animals exhibited any scored effects. Scratches and eschar were observed in all male and female animals persisting up until day 9. No oedema was observed in any test animals during the 14 day observation period.
Signs of Toxicity - Systemic	No signs of toxicity observed
Effects in Organs	No abnormalities were noted at necroscopy
Remarks - Results	Over the entirety of the test period, all animals showed gains in body weight.
CONCLUSION	The notified chemical is of low toxicity via the dermal route.
TEST FACILITY	BSL Bioservice (2012a)

B.2. Irritation – eye (in vitro)

TEST SUBSTANCE	Notified chemical (20% w/v dilution)
METHOD	OECD TG 437 Bovine Corneal Opacity and Permeability Test Method for Identifying Ocular Corrosives and Severe Irritants
Controls	Negative/Vehicle: 0.9% physiological sodium chloride Positive: 20% w/v Imidazole
Remarks - Method	GLP Certificate No significant protocol deviations Closed-chamber method Negative and positive control items were tested concurrently. Opacity was determined by an opacitometer.

RESULTS

Test material	*Mean opacities of triplicate tissues*	*Mean permeabilities of triplicate tissues*	*IVIS*
Vehicle control	3.33	0.016	0.57
*Test substance**	93.33	-0.014	93.13
*Positive control**	164.67	1.966	194.16

SD = Standard deviation; IVIS = in vitro irritancy score
*Corrected for background values

Remarks - Results	The positive control gave an in vitro irritation score that was reportedly within two standard deviations of the current historical mean confirming the validity of the test system. The study authors concluded that the test substance was a very severe eye irritant.
CONCLUSION	The notified chemical was a severe eye irritant under the conditions of the test.
TEST FACILITY	BSL Bioservice (2012b)

B.3. Skin sensitisation – mouse local lymph node assay (LLNA)

TEST SUBSTANCE	Notified chemical
METHOD	OECD TG 429 Skin Sensitisation: Local Lymph Node Assay EC Directive 2004/73/EC B.42 Skin Sensitisation (Local Lymph Node Assay)
Species/Strain	Mouse/ CBA/CaOlaHsd
Vehicle	Acetone/olive oil (4:1 v/v)
Remarks - Method	GLP Certificate No significant protocol deviations. A preliminary test was conducted with doses including 12.5%, 25% and 50% w/v. A concentration of 12.5% was subsequently chosen as the highest dose for investigation in the main test, based on the solubility of the test substance and reported excessive local irritation at the test sites of animals in the higher dosed groups. A concurrent positive control study was not run, but had been conducted previously in the test laboratory using P-Phenylenediamine.

RESULTS

Concentration (% w/w)	*Proliferative response (DPM/lymph node)*	*Stimulation Index (Test/Control Ratio)*
Test Substance		
0 (vehicle control)	471.9 (±89.9)	-
3.125	722.4 (±89.8)	1.5
6.25	1031.3 (±102.6)	2.2
12.5	1206.6 (±128.9)	2.6

Remarks - Results	No mortalities and no signs of systemic toxicity were noted in the test or control animals during the study. The results showed that the test substance at all concentrations elicited stimulation indices < 3 hence an EC3 value could not be derived. The results of radioactivity determination were supported by the ear thickness measurements, which showed no significant difference compared to the negative control.
CONCLUSION	There was no evidence of induction of a lymphocyte proliferative response indicative of skin sensitisation to the notified chemical.
TEST FACILITY	BSL Bioservice (2012c)

B.4. Genotoxicity – bacteria

TEST SUBSTANCE	Notified chemical

METHOD	OECD TG 471 Bacterial Reverse Mutation Test. EC Directive 2000/32/EC B.13/14 Mutagenicity – Reverse Mutation Test using Bacteria. Plate incorporation procedure/Pre incubation procedure
Species/Strain	*S. typhimurium*: TA1535, TA1537, TA98, TA100, TA102
Metabolic Activation System	S9 fraction from phenobarbital/β-naphthoflavone induced rat liver
Concentration Range in Main Test	a) With metabolic activation: 31.6–5,000 µg/plate b) Without metabolic activation: 31.6–5,000 µg/plate
Vehicle	DMSO
Remarks - Method	A preliminary test was conducted using TA98 and TA100 in the presence and absence of metabolic activation between 3.16–5,000 µg/plate (plate incorporation procedure). The results of the preliminary test formed part of Test 1.

RESULTS

Metabolic Activation	*Test Substance Concentration (µg/plate) Resulting in:*			
	Cytotoxicity in Preliminary Test	*Cytotoxicity in Main Test*	*Precipitation*	*Genotoxic Effect*
Absent				
Test 1	> 5,000	> 5,000	≥ 1,000	negative
Test 2		> 5,000	≥ 1,000	negative
Present				
Test 1	> 5,000	> 5,000	≥ 1,000	negative
Test 2		≥ 5,000	≥ 1,000	negative

Remarks - Results	Precipitation of test material was observed in all tester strains in both test 1 and 2 at concentrations of 1,000 µg/plate and higher in either the presence or absence of S9-mix. In test 1 no toxic effects of the test material were observed in any of the tester strains up to the highest dose group, with or without metabolic activation. Toxic effects were noted in test 2 for the tester strains TA 100 and TA 1535 in the presence of metabolic activation at a concentration of 5,000 µg/plate. No biologically significant increases in the frequency of revertant colonies were recorded for any of the bacterial strains, at any dose level, either with or without metabolic activation. The positive controls produced satisfactory responses, thus confirming the activity of the S9-mix and the sensitivity of the bacterial strains.
CONCLUSION	The notified chemical was not mutagenic to bacteria under the conditions of the test.
TEST FACILITY	BSL Bioservice (2012d)

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