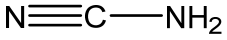
2	CAS No.: 420-04-2 (Cyanamide) 156-62-7 (Calcium cyanamide)	Substance: Cyanamide

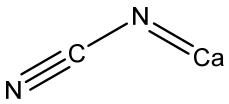
Chemical Substances Control Law Reference No.: 1-139 (Cyanamide)
1-121 (Calcium Cyanamide)
PRTR Law Cabinet Order No.: 1-137 (number after law revision*: 2-036)(Cyanamide)
1-77 (Calcium cyanamide)

Molecular formula:
CH_2N_2 (Cyanamide)
$CCaN_2$ (Calcium cyanamide)
Molecular weight:
42.04 (Cyanamide)
80.10 (Calcium cyanamide)

Structural formula:



Cyanamide



Calcium cyanamide

1. General information

The aqueous solubility of cyanamide is 7.75×10^5 mg/1,000 g (15°C), the partition coefficient (1-octanol/water) (log K_{ow}) is −0.72 (20°C) (pH=6.8), and the vapor pressure is 0.51 Pa (20°C). The biodegradability (aerobic degradation) is characterized by a BOD degradation rate of 0%. In addition, the hydrolysis half-lives were more than one year (pH=4, 7) (25°C) and 122 days (pH = 9) (25°C).

The aqueous solubility and partition coefficient (1-octanol/water) (log K_{ow}) of calcium cyanamide were not estimated using modeling because it dissociates in water to form cyanamide. The vapor pressure is 6.1×10^{-17} Pa (calculated value). The biodegradability (aerobic degradation) is 0% based on the quantity of CO_2 emitted. Further, hydrolyzability is characterized by residual ratios of 8.1% (after 2.5 min.), 6.3% (after 5 min.), and 4.4% (after 10 min.) (initial concentration: 200 mg/L) (23°C) (pH = 5).

Cyanamide was previously classified as a Class 1 Designated Chemical Substance under the PRTR Law, but it was removed from the classification by the Cabinet Order partially revising the Enforcement Order for the Act on the Assessment of Releases of Specified Chemical Substances in the Environment and the Promotion of Management Improvement promulgated on October 20, 2021, which came into force on April 1, 2023, and reclassified as a Class 2 Designated Chemical Substance.

The main uses of cyanamide are as an organic synthesis raw material, thiourea raw material, and pharmaceutical. It is also used as an agricultural chemical (plant growth regulator). Further, the production and import quantities in fiscal 2020 were not disclosed because the number of reporting businesses was less than two. The production and import category under the PRTR Law was more than 10 t.

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The main use of calcium cyanamide is as a raw material for fertilizer, agricultural chemicals, and industrial chemicals. Further, the production and import quantities in fiscal 2020 were not disclosed because the number of reporting businesses was less than two. The production and import category under the PRTR Law was more than 10 t.

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2. Exposure assessment

Total release of cyanamide to the environment in fiscal 2020 under the PRTR Law was approximately 8.2 t, of which 0.15 t or 2% were notified releases. The majority of notified releases to the atmosphere and public water bodies were to public water bodies. In addition, approximately 11 t was transferred to waste. The chemical industry was the sole source

of notified emissions. Including unnotified releases, most releases were to soil.

Total release of calcium cyanamide to the environment in fiscal 2020 under the PRTR Law was 0 t.

The reaction rate constant of this substance with OH radicals could not be obtained. Thus, predictions of proportions distributed to individual media could not be made.

The maximum expected concentration of exposure to humans via inhalation could not be defined because ambient atmospheric and indoor air quality data could not be obtained. Further, the mean annual value for atmospheric concentration in fiscal 2020 was calculated by use of a plume-puff model on the basis of releases to the atmosphere notified under the PRTR Law: this model predicts a maximum level of 0.00088 μg/m^3.

Data for potable water, groundwater, food, and soil to assess oral exposure could not be obtained. Thereupon, assuming ingestion solely from public freshwater bodies, a maximum predicted exposure of around 0.038 μg/kg/day was obtained.

The predicted environmental concentration (PEC) for cyanamide, which indicates exposure to aquatic organisms, was around 0.95 μg/L for public freshwater bodies and around 0.61 μg/L for seawater. Further, albeit data for a limited area, calculations for public freshwater bodies gave a maximum value of around 1.6 μg/L.

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3. Initial assessment of health risk

This substance severely irritates the eyes and the skin and irritates the respiratory tract as well. Inhalation of this substance will cause a cough and shortness of breath. Ingestion will cause burning sensation, sore throat and abdominal pain. Contact with the skin or the eyes will cause redness and pain. Calcium salt of this substance severely irritates the eyes and the respiratory tract. Inhalation will cause a cough, burning sensation, and sore throat, and ingestion will cause sore throat and burning sensation in the throat and the chest. Contact with the skin will cause redness. Contact with the eyes will cause redness and pain. There is a report on calcium salt of this substance that presented the lowest lethal dose of 571 mg/kg in humans.

Since not enough information was available on the carcinogenicity of the substance, the initial assessment was conducted based on information on its non-carcinogenic effects.

The NOAEL of 0.2 mg/kg/day for oral exposure (based on a decrease in mean corpuscular volume and mean corpuscular hemoglobin level), determined from toxicity tests in dogs, was deemed the lowest reliable dose and was identified as the 'non-toxic level' of the substance for oral exposure. The LOAEL of 148 mg/m^3 for inhalation exposure (based on suppression of body weight gain), determined from toxicity tests in rats, was adjusted according to exposure conditions to obtain 26 mg/m^3, and subsequently divided by a factor of 10 to account for uncertainty in using a LOAEL, and by another factor of 10 to account for extrapolation to chronic exposure. The calculated value of 0.26 mg/m^3 was deemed the lowest reliable concentration and was identified as the 'non-toxic level' of the substance for inhalation exposure.

Regarding oral exposure, assuming that the substance is absorbed via public freshwater bodies, the predicted maximum exposure level would be approximately 0.038 μg/kg/day. The MOE (Margin of Exposure) would be 530 which is calculated from the predicted maximum exposure level and the 'non-toxic level' of 0.2 mg/kg/day, and subsequently divided by a factor of 10 to account for extrapolation from animals to the humans. This would lead to the health risk judgment that no further work would be required at present. In addition, the MOE for reference would be 310 which is calculated from the estimated maximum exposure level of 0.064 μg/kg/day, according to data in a certain area on public freshwater bodies. Since exposure to the substance in environmental media via food is presumed to be limited, despite the lack of exposure level via food, including it in the calculation would not change the MOE significantly. Therefore, as a comprehensive judgment, no further work would be required at present.

Regarding inhalation exposure, due to the lack of identified exposure concentrations, the health risk could not be assessed. However, the maximum concentration (annual mean) in ambient air near the operators that are releasing a large amount of the substance was estimated to be 0.00088 μg/m^3, based on the releases to air reported in FY 2020 under the PRTR Law. The MOE for reference would be 30,000 which is calculated from the estimated concentration in ambient air and the 'non-

toxic level' of 0.26 mg/m^3, and subsequently divided by a factor of 10 to account for extrapolation from animals to humans. This would lead to the health risk judgment that no further work would be required at present, although it will be necessary to pay attention to the latest information on the emission source of this substance. Therefore, as a comprehensive judgment, no further work would be required at present.

Toxicity				Exposure assessment		MOE		Comprehensive judgment
Exposure Path	Criteria for risk assessment	Animal	Criteria for diagnoses (endpoint)	Exposure medium	Predicted maximum exposure dose and concentration			
Oral	'Non-toxic level*' 0.2 mg/kg/day	Dogs	Decrease in mean corpuscular volume and mean corpuscular hemoglobin level	Drinking water	- μg/kg/day	MOE	-	○
				Freshwater	0.038 μg/kg/day	MOE	530	
Inhalation	'Non-toxic level*' 0.26 mg/m^3	Rats	Suppression of body weight gain	Ambient air	- μg/m^3	MOE	-	○
				Indoor air	- μg/m^3	MOE	-	×

Non-toxic level *

- When a LOAEL is available, it is divided by 10 to obtain a NOAEL-equivalent level.
- When an adverse effect level for the short-term exposure is available, it is divided by 10 to obtain a level equivalent to an adverse effect level for the long-term exposure.

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4. Initial assessment of ecological risk

With regard to acute toxicity, the following reliable data were obtained: a 72-h of EC_{50} of 650 μg/L for growth inhibition in the cyanobacterium *Anabaena flos-aquae*, a 48-h EC_{50} of 2,680 μg/L for swimming inhibition in the crustacean *Daphnia magna*, and a 96-h LC_{50} of 38,600 μg/L for the fish *Cyprinus carpio* (carp). Accordingly, based on these acute toxicity values and an assessment factor of 100, a predicted no effect concentration (PNEC) of 6.5 μg/L was obtained.

With regard to chronic toxicity, the following reliable data were obtained: a 72-h NOEC of 110 μg/L for growth inhibition in the cyanobacterium *A. flos-aquae*, a 21-d NOEC of 100 μg/L for reproductive inhibition in the crustacean *D. magna*, and a 96-d NOEC 507 μg/L for growth inhibition in the fish *Oncorhynchus mykiss* (rainbow trout). Accordingly, based on these chronic toxicity values and an assessment factor of 10, a PNEC of 10 μg/L was obtained.

The value of 6.5 μg/L obtained from the acute toxicity to the cyanobacterium was used as the PNEC for this substance.

The PEC/PNEC ratio was 0.15 for freshwater bodies and 0.09 for seawater. Efforts to collect data are considered necessary in order to assess ecological risk.

Albeit data for a limited area, calculations for public freshwater bodies gave a maximum value of around 1.6 μg/L and the ratio of this value and PNEC was 0.2. Accordingly, based on a comprehensive review of the above findings, efforts to collect data are considered necessary Efforts to understand production and import quantities and trends in environmental releases are also considered necessary.

Hazard assessment (basis for PNEC)			Assessment coefficient	Predicted no effect concentration PNEC (μg/L)	Exposure assessment		PEC/ PNEC ratio	Comprehensive judgment
Species	Acute/ chronic	Endpoint			Water body	Predicted environmental concentration PEC (μg/L)		
Blue green algae	Acute	EC_{50} Growth inhibition	100	6.5	Freshwater	0.95	0.15	▲
					Seawater	0.61	0.09	

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5. Conclusions

	Conclusions		Judgment
Health risk	Oral exposure	No need for further work.	○
	Inhalation exposure	No need for further work.	○
Ecological risk	Requiring information collection.		▲

［Risk judgments］○: No need for further work ▲: Requiring information collection
■: Candidates for further work ×: Impossibility of risk characterization

*Note: Number after revision of law implemented on April 1, 2023