## SECTION-1: Identification of the substance / mixture and the company / undertaking

| | |
|---|---|
| **Catalogue Number** | CS-O-63533 |
| **Product Name** | Peroxyacetyl nitrate |
| **CAS No.** | 2278-22-0 |
| **Category** | Building Blocks |
| **Synonyms** | acetic nitric peroxyanhydride |
| **Brand** | Clearsynth Labs Ltd. |
| **Identified uses** | Laboratory Chemicals |
| **Uses advised against** | Not available |
| **Company** | Clearsynth Labs Ltd.<br>Mumbai, India |
| **Emergency Phone #** | +91-22-245045900 |
| **REACH No.** | Not available |

## SECTION 2: Hazards identification

**Disclaimer:** This is sample MSDS. Please email **sales@clearsynth.com** for more details.

### 2.1 Classification of the substance or mixture-Regulation (EC) No 1272/2008:

Not available

### 2.2 Label Elements

**Signal Word:** Not available

Not available

**Hazard Statement(s)**

| Code | Statement |
|---|---|
| Not available | Not available |

**Precautionary Statement(s)**

| Code | Statement |
|---|---|
| Not available | Not available |

## SECTION 3: Composition / information on ingredients

3.1 Substance

Component : Peroxyacetyl nitrate
CAS Number : 2278-22-0
Molecular Formula : C2H3NO5
Molecular Weight : 121.05
Parent Chemical : -
Synonyms : acetic nitric peroxyanhydride
Concentration : Not available

## SECTION 4: First aid measures

Not available

## SECTION 5: Firefighting measures

Not available

## SECTION 6: Accidental release measures

Not available

## SECTION-7: Handling and storage

Not available

## SECTION 8: Exposure controls / personal protection

Not available

## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

| Test | Result |
|---|---|
| Appearance | No data available |
| IR spectrum | No data available |
| pH | No data available |
| Solubility | No data available |

| Property | Value |
|---|---|
| a) Physical State | No data available |

| Property | Value |
|---|---|
| b) Color | No data available |
| c) Odor | No data available |
| d) pH | No data available |
| e) Vapour Pressure | No data available |
| f) Viscosity | No data available |
| g) Initial Boiling Point and boiling range | No data available |
| h) Melting Point / Freezing Point | No data available |
| i) Auto Ignition Temperature | No data available |
| j) Flash Point | No data available |
| k) Explosion Limit, Lower | No data available |
| l) Explosion Limit, Upper | No data available |
| m) Decomposition Temperature | No data available |
| n) Loss on Drying | No data available |
| o) Relative Density | No data available |
| p) Solubility (in DMSO) | No data available |
| q) Oxidizing Properties | No data available |

## SECTION 10: Stability and reactivity

Not available

## SECTION 11: Toxicological information

11.1 Information on toxicological effects
- Acute toxicity: /GENOTOXICITY/ A series of experiments was conducted in which Chinese hamsters ... were exposed to peroxyacetyl nitrate (PAN) in air at concentrations of approximately 3 ppm for up to 1 month and then examined for somatic mutations and chromosomal aberrations. Mutations were assayed by measuring the frequency of thioguanine-resistant lung fibroblasts (isolated de novo and cultured). Chromosomal aberrations were assayed by measuring the frequency of micronuclei in either the bone marrow (polychromatic erythrocytes) or the lungs (binucleate lung fibroblasts cultured in the presence of cytochalasin B). ... Although in each experiment the mutation frequencies for the test animals were higher than the corresponding controls, /they/ were not significantly different from the concurrent negative controls (P > .05) or the historical controls, except for experiment C. In experiment C, there was a significant regression of mutation frequency versus dose (P < 0.001) if all of the historical controls for pooled animals are included at zero dose. No reproducible evidence of chromosomal breakage was found in either lung or bone marrow. Thus, although PAN has been found to be a bacterial mutagen, /the authors/

did not find statistically significant evidence of mutagenicity in vivo. The toxicity of PAN limited the exposure concentration that could be used. ... /GENOTOXICITY/ Exposures of Salmonella typhimurium strain TA100 with and without S9 metabolic activation to low ppm levels of pure peroxyacetyl nitrate (PAN) in the gas phase were conducted. Measurements of the gas-phase PAN exposure concentration and the concentration of its decomposition products in surrogate test media led to a measured mutagenic activity of 34 +/- 5 revertants/umole. ...
- Skin corrosion/irritation: No data available.
- Serious eye damage/eye irritation: /SIGNS AND SYMPTOMS/ In humans, the lowest level causing eye irritation was 0.64 mg/cu m for 2 hr. /SIGNS AND SYMPTOMS/ Peroxyacetyl nitrate (PAN) is a ubiquitous air pollutant formed from NO(2) reacting with acetoxy radicals generated from ambient aldehydes in the presence of sunlight and ozone. It contributes to eye irritation associated with photochemical smog and is present in most urban air.
- Respiratory or skin sensitization: No data available.
- Germ cell mutagenicity: /GENOTOXICITY/ A series of experiments was conducted in which Chinese hamsters ... were exposed to peroxyacetyl nitrate (PAN) in air at concentrations of approximately 3 ppm for up to 1 month and then examined for somatic mutations and chromosomal aberrations. Mutations were assayed by measuring the frequency of thioguanine-resistant lung fibroblasts (isolated de novo and cultured). Chromosomal aberrations were assayed by measuring the frequency of micronuclei in either the bone marrow (polychromatic erythrocytes) or the lungs (binucleate lung fibroblasts cultured in the presence of cytochalasin B). ... Although in each experiment the mutation frequencies for the test animals were higher than the corresponding controls, /they/ were not significantly different from the concurrent negative controls (P > .05) or the historical controls, except for experiment C. In experiment C, there was a significant regression of mutation frequency versus dose (P < 0.001) if all of the historical controls for pooled animals are included at zero dose. No reproducible evidence of chromosomal breakage was found in either lung or bone marrow. Thus, although PAN has been found to be a bacterial mutagen, /the authors/ did not find statistically significant evidence of mutagenicity in vivo. The toxicity of PAN limited the exposure concentration that could be used. ... /GENOTOXICITY/ Exposures of Salmonella typhimurium strain TA100 with and without S9 metabolic activation to low ppm levels of pure peroxyacetyl nitrate (PAN) in the gas phase were conducted. Measurements of the gas-phase PAN exposure concentration and the concentration of its decomposition products in surrogate test media led to a measured mutagenic activity of 34 +/- 5 revertants/umole. ...
- Carcinogenicity: No data available.
- Reproductive toxicity: /PLANTS/ ... Peroxyacetyl nitrate (PAN) has a well-documented history as damaging to vegetation. There have been few long-term experimental studies despite the field evidence for damaging effects. Early studies in California have been followed by more recent data from east Asia, but there is still a dearth of information on the potential for effects of PAN and related peroxyacyl nitrates on vegetation typical of regions around tropical and sub-tropical cities where PAN pollution is increasingly important. ... Although reproductive processes (flowering, seed production) appear to be most sensitive, there have been no experimental studies on subsequent seed viability and the consequences at the ecosystem level of changes to plant phenology. ...
- STOT-single exposure: No data available.
- STOT-repeated exposure: /ALTERNATIVE and IN VITRO TESTS/ Peroxyacetyl nitrate (PAN) ... induced apoptosis in human leukemia HL-60, human chronic myelogenous leukemia K-562, and mouse monocyte-macrophage RAW 264.7 cell lines. In the HL 60 cells, characteristic apoptosis morphology could be observed 4 hr after the cells were treated with 50 uM PAN. Exposure of HL-60 cells to increasing concentrations of PAN (from 1 uM to 100 uM) confirmed the concentration dependence of apoptosis as evidenced by DNA fragmentation in HL-60 cells, chromatin condensation by acridine-orange staining, and the appearance of the DNA apoptotic peak in flow cytometry. During apoptosis in HL-60 cells, 3-nitrotyrosine and 3,5-dinitrotyrosine were detected by high-performance liquid chromatography and liquid chromatography-mass spectrometry-mass spectrometry. ... Moreover, exogenous superoxide dismutase promoted PAN-induced apoptosis, and in contrast, a combination of superoxide dismutase and catalase suppressed this apoptosis. ... The formation of H2O2 produced from the dismutation of PAN-elicited

superoxide anion contributed to the apoptotic mechanism in HL-60 cells through ROS pathways. ... /LABORATORY ANIMALS: Subchronic or Prechronic Exposure/ Male and female WIstar rats were exposed to peroxyacetyl nitrate (PAN) for 6 hours/day, 5 days/week for either 4 or 13 weeks. PAN concentrations used in the 4 week study were 0, 0.9, 4.1, or 11.8 ppm; concentrations used in the 13 week study were 0, 0.2, 1.0 or 4.6 ppm. In the 4 week study, exposure to 11.8 ppm caused elevated mortality, hematocrit values, red blood cell counts and lung weight. In addition, exposure resulted in abnormal behavior, growth retardation, severe inflammation, epithelial metaplasia and hyperplasia in the respiratory tract. Minimal behavioral disturbance, transient growth retardation, slightly increased lung weights and slight histopathological changes in the respiratory tract were noted at 4.1 ppm. No treatment related effects were noted at 0.9 ppm. Exposure to 4.6 ppm in the 13 week study resulted in changes similar to those found at 11.8 ppm in the 4 week study, with the exception that elevated mortality was not observed. No treatment-related effects exhibiting a dose-response were observed at 1.0 ppm.
- Aspiration hazard: No data available.

Likely routes of exposure
- LC50 Strain A male mice (9 wks) inhalation 718-743 mg/cu m (2 hr)

Symptoms related to the physical, chemical and toxicological characteristics
- /HUMAN EXPOSURE STUDIES/ The metabolic and pulmonary function effects were investigated in 10 nonsmoking, young adult men who were exposed for 2 hr (20 degrees C...) to 4 conditions: (1) filtered air (FA), (2) 0.30 ppm peroxyacetyl nitrate (PAN), (3) 0.45 ppm ozone (O3), and (4) 0.45 ppm O3 + 0.30 ppm PAN (PAN/O3). The subjects alternated 15-min periods of rest and 20-min periods of bicycle ergometer exercise at a work load predetermined to elicit a ventilatory minute volume (VE) of 27 L/min (BTPS). Functional residual capacity (FRC) was determined pre- and postexposure. Forced vital capacity (FVC) was determined before and after exposure, and 5 min after each exercise period. Heart rate was monitored throughout the exposure, and (VE), oxygen uptake (VO2), respiratory rate (fR), and tidal volume (VT) were measured during the last 2 min of each exercise period. There were no changes in any variable consequent to FA or PAN exposure. The only metabolic changes to occur because of O3 and PAN/O3 exposure were a decrease in VT, a concomitant increase in fR, and consequently no change in VE. Both O3 and PAN/O3 induced significant ($p < 0.05$) decrements in FVC, FEV1.0, FEV2.0, FEV3.0, FEF25-75%, IC, ERV, and TLC. The decrements after PAN/O3 exposure averaged 10% greater than the decrements after O3 exposure. ...

## SECTION 12: Ecological information

Not available

## SECTION 13: Disposal considerations

Not available

## SECTION 14: Transport information

Not available

## SECTION 15: Regulatory information

Not available

## SECTION 16: Other information

Not available

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