I U C L I D

D a t a S e t

Existing Chemical	ID: 1646-75-9
CAS No.	1646-75-9
EINECS Name	2-methyl-2-(methylthio)propionaldehyde oxime
EC No.	216-709-5
Molecular Formula	C5H11NOS

Producer Related Part

Company:	TNO Quality of Life
Creation date:	23-SEP-2005

Substance Related Part

Company:	TNO Quality of Life
Creation date:	23-SEP-2005

Memo:	SIDS ADO (final)
Printing date:	16-JAN-2006
Revision date:	
Date of last Update:	**16-JAN-2006**
Number of Pages:	**35**
Chapter (profile):	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile):	Reliability: without reliability, 1, 2, 3, 4
Flags (profile):	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 Applicant and Company Information

Type: manufacturer
Name: other: Honeywell International Inc.
Street: 101 Columbia Road
Town: NJ 07962 Morristown
Country: United States

23-SEP-2005

1.0.2 Location of Production Site, Importer or Formulator

Type: manufacturer
Name of Plant: Hopewell Virginia plant

23-SEP-2005

1.0.3 Identity of Recipients

Name of recip.: unknown

Remark: Aldicarb oxime (ADO) is used as an agricultural intermediate in the production of carbamate pesticides. The substance is sold to one customer who uses it at only one site.
29-NOV-2005

1.0.4 Details on Category/Template

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1.1.0 Substance Identification

Mol. Formula: C5H11NOS
Mol. Weight: 133

23-SEP-2005

1.1.1 General Substance Information

Purity type: typical for marketed substance
Substance type: organic
Physical status: liquid
Purity: > 99 - % w/w
Colour: clear, colourless

Remark: pH of the substance is 7. The substance has no significant impurities and no additives are present.
23-SEP-2005

1.1.2 Spectra

-

1.2 Synonyms and Tradenames

2-(methylthio)isobutyraldehyde oxime

23-SEP-2005

2-methyl-2-(methylthio)propionaldehyde oxime

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2-methyl-2-(methylthio)propionaldoxime

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Aldicarb Oxime: ADO

23-SEP-2005

propanal, 2-methyl-2-(methylthio)-, oxime

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propionaldehyde,2-methyl-2-(methylthio)-,oxime

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Temik oxime

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1.3 Impurities

Purity type: other: no significant impurities

06-OCT-2005

1.4 Additives

Purity type: other: None

06-OCT-2005

1.5 Total Quantity

Remark: Total amount of substance produced is 1 to 5 MM lbs/yr.
06-OCT-2005

1.6.1 Labelling

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1.6.2 Classification

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1.6.3 Packaging

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1.7 Use Pattern

Type: industrial
Category: Agricultural industry

Remark: Chemical Intermediate in the production of carbamate pesticides, used only at one site.
06-OCT-2005

1.7.1 Detailed Use Pattern

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1.7.2 Methods of Manufacture

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1.8 Regulatory Measures

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1.8.1 Occupational Exposure Limit Values

Type of limit: other

Remark: The substance is primarily used by industrial workers experienced in the handling of substances of greater toxicity. Significant airborne levels of the substance should not occur due to its low vapor pressure. Honeywell has established PEL of 10 ppm (54.3 mg/m3) as an 8 hour TWA.
19-OCT-2005 (20)

1.8.2 Acceptable Residues Levels

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1.8.3 Water Pollution

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1.8.4 Major Accident Hazards

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1.8.5 Air Pollution

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1.8.6 Listings e.g. Chemical Inventories

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1.9.1 Degradation/Transformation Products

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1.9.2 Components

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1.10 Source of Exposure

Source of exposure: Human: exposure by production
Exposure to the: Substance

Remark: ADO is produced at only one Honeywell site, for one customer. The synthesis of the product is conducted in a sealed system minimizing employee exposure.

As exposures are very low (relative to the Honeywell PEL of 10 ppm), monitoring at the production site has been conducted infrequently. The results form this monitoring confirm that exposures are low.

Date	Personal (#)	Area (#)
Aug.-Nov 1977	<0.45 ppm (8)	<0.1 ppm (16)
Feb-April 1978	<0.29 ppm (8)	
Sept 1978	<0.04 ppm (2)	<0.02 ppm (5)
Oct. 1978	<0.05 ppm (3)	<0.12 ppm (4)
May 1985	0.05 ppm (1)	0.01 ppm (1)

23-SEP-2005 (21)

1.11 Additional Remarks

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1.12 Last Literature Search

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1.13 Reviews

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2.1 Melting Point

Value: = 21 degree C

Method: other
GLP: no data
Test substance: no data

Reliability: (2) valid with restrictions (9) (20)
23-SEP-2005

Deleted: (4) not assignable

2.2 Boiling Point

Value: = 210 degree C

Method: other
GLP: no data
Test substance: no data

Remark: The substance boils with partial decomposition.
Reliability: (2) valid with restrictions (9) (20)
23-SEP-2005

Deleted: (4) not assignable

2.3 Density

Value: = 1.05 g/cm³

Method: other: specific gravity
GLP: no data
Test substance: no data

Reliability: (2) valid with restrictions (9) (20)(21a)
23-SEP-2005

Deleted: (4) not assignable

2.3.1 Granulometry

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2.4 Vapour Pressure

Value: < .1 at 20 degree C

Method: other (measured)
GLP: no data
Test substance: no data

Reliability: (2) valid with restrictions (9) (20)(21a)
23-SEP-2005

Deleted: (4) not assignable

2.5 Partition Coefficient

Partition Coeff.: octanol-water
log Pow: 0.75
Method: EPIWIN 3.12
GLP: no data
Test substance: no data

Reliability: (2) calculated value, therefore valid with restrictions
23-SEP-2005 (5)

Deleted: ca. 15.1¶
Deleted: other (calculated)
Deleted: (4) not assignable

2.6.1 Solubility in different media

Solubility in: Water
Value: = 2.5 other: wt% at 22 degree C

Method: other
GLP: no data
Test substance: no data

Remark: Henry's Law Constant
Results: 7.12e-007 atm.-m3/mole
Method: calculated from VP: 0.1 mm Hg
Water solubility: 2.5 e+004 ppm
HENRYWIN v3.10

Reliability: (2) calculated value, therefore valid with restrictions
23-SEP-2005 (20)

Deleted: (4) not assignable

Solubility in : Water
Value: = 2.7 wt % at ~23˚C
Method: HPLC
GLP no
Test Substance: 92.6% as determined by HPLC
Remark A saturated solution of ADO was prepared by stirring an excess of ADO in well water at ~ 23˚C for three hours and letting it settle for 1 hour. The clear supernatant was decanted off into a clean gloss tube and sealed with a Teflon-lined screw cap. Reverse-phase chromatography was preformed using an LDC Constametric II HPLC system with a Whatman Parisil PxS 10/25 ODS-2 column. The solvent was acetonitrile/water.
Reliability: 1 (original report reviewed)
(3)

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2.6.2 Surface Tension

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2.7 Flash Point

Value: = 118 degree C
Type: open cup

Method: other
GLP: no data
Test substance: no data

Reliability: (2) valid with restrictions

Deleted: (4) not assignable

2.8 Auto Flammability

Value: = 285 degree C

Method: other
GLP: no data
Test substance: no data

Reliability: (4) not assignable
23-SEP-2005 (20)

2.9 Flammability

Result: non flammable

Method: other
GLP: no data
Test substance: no data

Reliability: (4) not assignable
23-SEP-2005 (20)

2.10 Explosive Properties

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2.11 Oxidizing Properties

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2.12 Dissociation Constant

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2.13 Viscosity

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2.14 Additional Remarks

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3.1.1 Photodegradation

Type of measurement: other

Remark: Model AopWin v1.91
Hydroxyl Radical Reaction:
Overall OH Rate Constant = 4.3506 e-12 cm3/molecule-sec
Half-life = 2.459 days (12-hr day; 1.5 e6 OH/cm3)

Soil Adsorption (PCKOCWIN v1.66):
Koc = 380.8 log Koc = 2.581
Reliability: (1) valid without restriction

3.1.2 Stability in Water

Type: abiotic

Method: other: HPLC analysis of saturated solution
GLP: yes
Test substance: purity by analysis 97.4%
Remark: A saturated solution of ADO was prepared by stirring excess ADO in well water for three hours and allowing it to settle for one hour. The supernatant was evaluated by maintaining the solution for 15 days and analyzing by HPLC at periodic intervals.
Result: The substance was stable for at least 15 days
Reliability: (2) valid with restrictions
23-SEP-2005 (3)

Type: abiotic
t1/2 pH4: > 5 day(s) at 50 degree C
t1/2 pH7: > 5 day(s) at 50 degree C
t1/2 pH9: > 5 day(s) at 50 degree C
Deg. products: not measured

Method: OECD Guide-line 111 "Hydrolysis as a Function of pH"
GLP: yes
Test substance: other TS

Method: Aqueous solutions of the test substance in buffer solutions (pH 4.0, 7.0 and 9.0) were kept at 50°C for 5 days. The concentration of the substance was determined at days 0, 1 and 5 using the HPLC. The percentage hydrolysis was determined after 5 days at each pH.
Result: The reproducibilty and repeatability of the analytical method for the measurment of the test substance was determined. The recoveries measured were between 95.9 and 102%. The reproducibility (RSD in the measured concentration of 5 validation samples) of this method was 0.48% for pH 4.0, 1.6% for pH 7.0 and 0.82% for pH 9.0.

The % hydrolysis of ADO measured after incubation at 50°C after 5 days was -1.3%, 4/6% and 7.6% at pH 4.0, 7.0 and 9.0, respectively. Since the % hydrolysis of ADO in all buffer solutions is less than 10 after incubation at 50°C for 5 days, ADO is considered to be hydrolytically stable at pH 4.0, 7.0 and 9.0.

Test substance: The test substance tested has a purity of 98.8%.
Reliability: (1) valid without restriction
16-JAN-2006 (1)

3.1.3 Stability in Soil

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3.2.1 Monitoring Data (Environment)

Type of measurement: other

Remark: Model AopWin v1.91
Hydroxyl Radical Reaction:
Overall OH Rate Constant = 4.3506 e-12 cm3/molecule-sec
Half-life = 2.459 days (12-hr day; 1.5 e6 OH/cm3)

Soil Adsorption (PCKOCWIN v1.66):
Koc = 380.8 log Koc = 2.581
Reliability: (1) valid without restriction
23-SEP-2005

3.2.2 Field Studies

-

3.3.1 Transport between Environmental Compartments

Type: fugacity model level III
Method: other

Remark: Input data:
Water solubility 25,000 mg/L
Vapor pressure: 0.1 mm Hg
Log Kow = 15.1
Boiling Point: 210°C
Melting point: 21°C

Level III Fugacity Model:

	Percent	Half-life	Emissions
Air	1.92%	59 hr.	1000 kg/hr
Water	6.97%	360 hr.	1000 kg/hr
Soil	29.2%	360 hr.	1000 kg/hr
Sediment	61.9%	1.44 e3	0

Persistence Time: 669 hr.
Reliability: (1) valid without restriction
23-SEP-2005

3.3.2 Distribution

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3.4 Mode of Degradation in Actual Use

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3.5 Biodegradation

Result: under test conditions no biodegradation observed

Method: other: Static shake flask-CO2 evolution
GLP: yes
Test substance: other TS

Method: An acclimated mixed culture inoculum derived from activated sludge and soil was exposed to 10 mg/L organic carbon of ADO for 28 days at 23 degree C (SD 4 degree C). Evolution of CO2 and removal of soluble organic carbon were evaluated.
Result: Cumulative 28 day percentage CO2 evolutions was 2.62% and cumulative 28 day soluble organic carbon removal was <1.0%.
Test substance: Purity: 97.4%
Reliability: (1) valid without restriction
29-NOV-2005 (8)

3.6 BOD5, COD or BOD5/COD Ratio

-

3.7 Bioaccumulation

Species: other

Remark: There are no data available. The given LogPOw value (15.1) is not considered reliable and the substance is not biodegradable. A reliable LogPow must be made available.
29-NOV-2005

3.8 Additional Remarks

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AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

Type: static
Species: Lepomis macrochirus (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no data
LC50: = 275 calculated
Limit Test: no

Method: other
GLP: yes
Test substance: other TS purity by analysis 97.4%

Method: Bluegill sunfish were exposed to five nominal ADO concentrations (66, 102,158,243 and 374 mg/L) for 96 hours at 22 degree C under static test conditions.
Result: The acute lethality threshold concentration at 96 hours was between 102 and 158 mg/L. An NOEL was < 66 mg/L. The fish were exposed in groups of 10 each in 15 L aquaria. They were observed at 1-, 24-, 28- 72- and 96-hours. Analytical analysis over time demonstrated that the ADO was stable in the aqueous media (no degredation over 28 days, concentrations were 2.84% and 2.88% for the concentrated stock solution.

Nominal Concentration (mg/L_)	%Mortality @ 1-hr	%Mortality @ 24-hr	%Mortality @ 48-hr	%Mortality @ 72-hr	%Mortality @ 96-hr
374	0	90	90	100	100
243	0	0	0	0	0
158	0	0	0	0	10
102	0	0	0	0	0
66	0	0	0	0	0
Control	0	0	0	0	0

Test substance: Purity: 97.4%
Reliability: (1) valid without restriction
29-NOV-2005 (2)

Type: static
Species: Salmo gairdneri (Fish, estuary, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no data
LC50: = 28 calculated
NOEL : = 16 measured/nominal
Limit Test: no

Method: other
GLP: yes
Test substance: other TS purity by analysis 97.4%

Method: Rainbow trout were exposed to five nominal ADO concentrations (16, 27, 44, 75 and 125 mg/L) for 96 hours at 12 degree C under static test conditions. The fish were exposed in groups of 10 each in 15 L aquaria. They were observed at 1-, 24-, 28- 72- and 96-hours. Analytical

analysis over time demonstrated that the ADO was stable in the aqueous media (no degredation over 28 days, concentrations were 2.84% and 2.88% for the concentrated stock solution.

Result: The acute lethality threshold concentration at 96 hours was between 16 and 27 mg/L.

Nominal Concentration (mg/L_)	%Mortality @ 1-hr	%Mortality @ 24-hr	%Mortality @ 48-hr	%Mortality @ 72-hr	%Mortality @ 96-hr
125	0	100	100	100	100
75	0	90	90	90	100
44	0	70	90	90	90
27	0	20	40	50	60
16	0	0	0	0	0
Control	0	0	0	0	0

Test substance: Purity: 97.4% (sample CMA #8137-63A)
Reliability: (1) valid without restriction
27-OCT-2005 (7)

23-SEP-2005

4.2 Acute Toxicity to Aquatic Invertebrates

Type: static
Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** no data
NOEC: = 137 measured/nominal
EC50: = 343 calculated
Limit Test: no

Method: other
GLP: yes
Method: Daphnids were exposed to five nominal ADO concentrations (96, 137, 196, 280 and 400 mg/L) for 48 hours under static test conditions.
Test substance: Purity: 97.4%
Results:
The Daphnia were exposed in groups of 20 each in 8 ounce sealed flasks. They were observed for 48 hours. Analytical analysis over time demonstrated that the ADO was stable in the aqueous media (no degredation over 15 days, concentrations were 2.67% and 2.72% for the concentrated stock solution.

Immobilization at Various Time intervals up to 48-Hours

Nominal Concentration (mg/L)	1-hr	3-hr	5-hr	24-he	30-hr	48-hr
400	95	95	100	75	75	95
280	25	10	0	0	0	0
196	0	0	0	0	0	0
137	0	0	0	0	0	0
96	0	0	0	0	0	0
Control	0	0	0	0	0	0

Reliability: (1) valid without restriction
29-NOV-2005 (4)

4.3 Toxicity to Aquatic Plants e.g. Algae

Species: Selenastrum capricornutum (Algae)
Endpoint: growth rate
Exposure period: 72 hour(s)
Unit: mg/l **Analytical monitoring:** yes
Limit Test: no

Method: OECD 201 and EU C.3
Year: 1992
GLP: yes
Test substance: other TS

Method: Concentrations tested were: 10, 33, 58, 103, 329 mg/L (nominal). At the start of the test, the concentrations were found to be 92-104% of the nominal concentration (mean value 98%) and at the end of the test, the measured concentrations were found to be 95-101% (mean value 98%). Since the concentrations decreased by less than 20% nominal concentrations were used to report the test results.
Result: NOEC: 33 mg/L

NEC: 14.1 mg/L (95% confid.8.1-20.2)
ErC10: 140 mg/L
ErC50: > 329 mg/L (95% confid.640-930;extrapolated 770)
ErC90: > 329 mg/L (extrapolated: 4100)
EbC10: 27 mg/L (range 10-33)
EbC50: 180 mg/L (range 100-329)
EbC90: > 329 mg/L

Reliability: (1) valid without restriction
06-OCT-2005 (16)

4.4 Toxicity to Microorganisms e.g. Bacteria

Type: other
Species: activated sludge
Exposure period: 5 hour(s)
Unit: mg/l **Analytical monitoring:** no data
IC50 : > 5000 measured/nominal

Method: other: STM, ESL-009, Microbial Toxicity (IC50)-Lockhart method, respiration rate
GLP: yes
Test substance: other TS purity by analysis 97.4%

Method: An activated sludge inoculum was exposed to four nominal ADO concentrations (5, 50, 500 and 5000 mg/L) at 27 degree C.
Result: Concentrations of ADO of 500 mg/L or less had no inhibitory effect on microbial metabolism. Approximately 20% of microbial metabolism as measured by 14CO2 evolution was observed at 5000 mg/L. Therefore, an IC50 was not reached.
Test substance: Purity: 97.4%
Reliability: (1) valid without restriction
06-OCT-2005 (6)

4.5 Chronic Toxicity to Aquatic Organisms

4.5.1 Chronic Toxicity to Fish

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4.5.2 Chronic Toxicity to Aquatic Invertebrates

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TERRESTRIAL ORGANISMS

4.6.1 Toxicity to Sediment Dwelling Organisms

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4.6.2 Toxicity to Terrestrial Plants

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4.6.3 Toxicity to Soil Dwelling Organisms

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4.6.4 Toxicity to other Non-Mamm. Terrestrial Species

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4.7 Biological Effects Monitoring

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4.8 Biotransformation and Kinetics

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4.9 Additional Remarks

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5.0 Toxicokinetics, Metabolism and Distribution

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5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity

Type: LD50
Species: rat
Strain: Wistar
Sex: male
No. of Animals: 15
Vehicle: no data
Doses: 2.0, 1.0, 0.5 mL/kg
Value: = 746 mg/kg bw

Method: other
GLP: no
Test substance: no data

Result: Mortality was 5/5, 3/5 and 2/5, respectively. Rats became prostrate with heavy breathing 10 minutes post dose. Deaths occurred within 30 minutes at the two highest dose levels and within 3 hours at the low dose.
Reliability: (2) valid with restrictions
23-SEP-2005 (11)

Type: LD50
Species: rat
Strain: other: Harlan-Wistar
Sex: no data
Vehicle: no data
Doses: 0.707 mL/kg (742 mg/kg)
Value: = 742 mg/kg bw

Method: other
GLP: no
Test substance: no data

Method: Undiluted sample of ADO designated for 7-day feeding study (see below) was tested for acute peroral intubation toxicity using nonfasted rats weighing 98-120 grams. No additional details were given in the report. Dose levels were not specified in the report.
Result: Rats were reported to have unsteady gait and piloerection, were prostrate within 5 minutes, and death, when it occurred, was within 0.5 to 3 hours.
Reliability: (2) valid with restrictions
23-SEP-2005 (12)

Type: LD50
Species: rat
Strain: Wistar
Sex: male
No. of Animals: 10
Vehicle: no data
Doses: 1.0, 0.5 mL/kg
Value: = 809 mg/kg bw

Method: other
GLP: no
Test substance: no data

Method: Undiluted sample of ADO was administered to groups of 5 male rats weighing 90-120 grams at dose levels of 1.0 and 0.5 mL/kg.
Result: Four of five animals died at the high dose while no deaths occurred at the low dose. High dose animals were observed to be prostrate within minutes after dosing with death occurring soon after. Gross pathological examination (apparently of the animals that died) found congestion throughout the thoracic and abdominal viscera. The LD50 was set at 0.77 mL/kg (809 mg/kg).
Reliability: (2) valid with restrictions
29-NOV-2005 (10)

Type: LD50
Species: rat
Strain: other: Harlan-Wistar
Sex: male
Vehicle: other: corn oil
Doses: 2380 mg/kg
Value: = 2380 mg/kg bw

Method: other
GLP: no
Test substance: no data

Method: Male rats (number not specified) weighing 90-120 grams were dosed by gavage with ADO in corn oil.
Result: LD50 calculated by the moving average method is reported. Higher LD50 than reported for undiluted ADO likely due to reduced absorption from the oil vehicle related to high solubility in oil as shown by partition coefficient for ADO.
Reliability: (2) valid with restrictions
23-SEP-2005 (14)

5.1.2 Acute Inhalation Toxicity

Type: LC50
Species: rat
Strain: other: Crl:CD (SD) BR
Sex: male/female
No. of Animals: 40
Vehicle: no data
Doses: 0.67, 1.12, 2.55, 4.91 mg/L
Exposure time: 4 hour(s)
Value: = 1230 mg/m³

Method: other
GLP: yes
Test substance: no data

Method: Four groups of 5 male and 5 female rats received whole-body inhalation exposures to aerosol atmospheres of ADO having a mass median diameter of 2.85 micrometers and geometric standard deviation of 1.93. Gravimetric time-weighted average concentrations were 0.67, 1.12, 2.55 and 4.91 mg/L. The animals were followed for 14 days following the exposure.
Remark: Exposures of the high and low exposure groups were for 3.5 hours rather than 4 hours due to insufficient test material. Study director recalculated original LC50 of 1,560 mg/m3 assuming 2 and 1 additional deaths would have occurred in the high and low exposure groups , respectively, with an additional 30 min. of exposure.
Result: Mortality occurred at all exposure levels tested. Females were slightly more sensitive than males. Major clinical signs included prostration, ataxia, tremors, irregular breathing, salivation and lacrimation. Animals dying exhibited gross abnormalities primarily of the lungs (red discoloration).
Reliability: (2) valid with restrictions
23-SEP-2005 (24)

Type: other: LC50 limit test
Species: rat
Strain: other: Sherman-Wistar
Sex: no data
No. of Animals: 10
Vehicle: no data
Doses: 2 mg/L
Exposure time: 1 hour(s)
Value: > 2 mg/l

Method: other
GLP: no
Test substance: no data presumed to be >95% based on analyses of other Allied samples.

Method: Acute, whole body inhalation. Performed according to criteria specified in Paragraph 191.1 (c) (2) and (f) (2) of the Final Order, Enforcement Regulations, Federal Register, vol 26, no 155, p. 7336, 12 August, 1961).

Ten rats (sex not specified) with an average weight of 285 grams were exposed to ADO for one hour in a 72 liter glass chamber. Air flow was 10 L/min. ADO was generated as a fine aerosol. Nominal concentration was 2 mg/L.

Result: No deaths occurred. Animals appeared docile and stressed immediately after the exposure with full recovery in 24 hours. No other information given in this one page report.

Reliability: (2) valid with restrictions

23-SEP-2005 (17)

Type: other
Species: rat
Strain: Wistar
Sex: no data
No. of Animals: 12
Vehicle: no data
Doses: saturated vapour
Exposure time: 8 hour(s)

Method: other
GLP: no
Test substance: other TS presumed to be >95% based on analysis of other Allied samples.

Method: Saturated vapor was generated by spreading 50 grams of chemical over 200 cm2 area on a shallow tray placed near the top of a 120-liter glass chamber which was subsequently sealed for at least 16 hours with intermittent agitation with a fan. Rats were introduced into the chamber in a gasketed drawer-type cage designed and operated to minimize vapor loss (method described in earlier report from this lab, assumed method was unchanged for this study). Each of the two samples ADO were tested separately. In each study, 6 animals were exposed to the saturated vapor for 8 hours.

Result: The ADO sample of 92.7% purity caused no mortality but produced the following signs of toxicity: eyes closed within 30 minutes, lacrimation within 60 minutes, slight coordination loss within 90 minutes. Signs were no longer present after 4 hours of the 8 hour exposure. The ADO sample of 99.25% purity caused no deaths but produced signs of closed eyes within 30 minutes, slight gasping within 60 minutes, slight coordination loss within 90 minutes. Signs were no longer present after 4 hours of the 8 hour exposure. The report concludes that the signs of toxicity observed may have been due to the presence of impurities that gradually reduced in concentration either through loss or chemical reactions during the course of the exposure.

Test substance: Purity (2 samples) : 92.7% and 99.25%

Reliability: (3) invalid

29-NOV-2005 (13)

23-SEP-2005

5.1.3 Acute Dermal Toxicity

Type: LD50
Species: rabbit
Strain: other: albino
Sex: no data
No. of Animals: 25
Vehicle: no data
Doses: 0.02, 0.2, 0.43, 0.928, 2.0 g/kg
Value: = 1900 mg/kg bw

Method: other: 16 CFR 1500.40
GLP: no
Test substance: 97.4% based on analysis

Result: Mortality occurred in all groups except at 0.928 mg/kg. The dose response was "U-shaped" (2/5, 1/5, 1/5, 0/5 and 3/5, respectively). No gross pathological effects were observed at necropsy. No additional information is provided in the single page report.
Reliability: (2) valid with restrictions
23-SEP-2005 (18)

Type: other: limit test
Species: rabbit
Strain: New Zealand white
Sex: male
No. of Animals: 4
Vehicle: other: none
Doses: 210 mg/kg (0.2 mL/kg)
Value: = 210 mg/kg bw

Method: other
GLP: no
Test substance: no data
Method: Four male rabbits were exposed dermally to ADO at a dose of 0.2 mL/kg for 24 hours under Vinylite covering (occlusive).
Result: Mortality occurred in one of the rabbits (25% of the animals exposed). No signs or symptoms were reported. Necropsy was not performed on the dead rabbit because of autolysis.
Reliability: (2) valid with restrictions
19-OCT-2005 (10)

5.1.4 Acute Toxicity, other Routes

Type: LD50
Species: mouse
Strain: other: albino
Sex: male
No. of Animals: 5
Vehicle: water
Doses: 100 mg/kg
Route of admin.: i.v.
Exposure time: 24 hour(s)
Value: < 100 mg/kg bw

Method: other: range finding study
GLP: no
Test substance: no data

Method: 5 male mice weighing 24 to 28 grams were injected with ADO as a 1% aqueous solution.
Result: All of the animals died within 24 hours of the injection. Reported signs included marked depression and gasping. Eye and pinna reflexes appeared normal.
Reliability: (3) invalid
19-OCT-2005 (10)

5.2 Corrosiveness and Irritation

5.2.1 Skin Irritation

Species: rabbit
Concentration: undiluted
Exposure: Occlusive
Exposure Time: no data
No. of Animals: 5
Vehicle: other: none
Result: moderately irritating

Method: other
GLP: no
Test substance: no data

Method: The substance was applied undiluted to the clipped intact skin of the belly of 5 rabbits. Exposure was not occluded (uncovered).
Result: ADO produced moderate erythema on 3 animals and moderate to marked capillary injection on 2 others. Test scored as grade 4 based on a ten point system.
Reliability: (2) valid with restrictions
27-OCT-2005 (10)

5.2.2 Eye Irritation

Species: rabbit
Concentration: undiluted
Dose: other
Exposure Time: unspecified
No. of Animals: 5
Vehicle: other: propylene glycol
Result: highly corrosive

Method: other
GLP: no
Test substance: no data

Method: Single exposure of undiluted ADO (0.005 mL) or 0.5 mL of a 5% or 15% ADO in propylene glycol was introduced into conjunctival sac. Observed one hour and 24 hours after exposure. Total number of animals used not specified.
Result: Undiluted ADO (0.005 mL) or 0.5 mL of a 15% ADO in propylene glycol caused moderately severe corneal necrosis. 5% ADO caused no injury in 2 eyes and only a trace of diffuse corneal necrosis in a third. Some eyelid irritation was also noted. Test scored as grade 8 based on a ten point system.
Reliability: (2) valid with restrictions
19-OCT-2005 (10)

23-SEP-2005

5.3 Sensitization

Type: other

Remark: No data available.
23-SEP-2005

5.4 Repeated Dose Toxicity

Type: Sub-chronic
Species: rat **Sex:** male/female
Strain: Crj: CD(SD)
Route of administration: oral feed
Exposure period: 13 weeks
Frequency of treatment: continuous
Doses: 5, 25, 125 mg/kg
Control Group: yes
NOAEL: = 120.2 mg/kg
LOAEL: > 120.2 mg/kg

Method: other
GLP: no
Test substance: no data (assumed to be >95% based on other Allied sample analyses)

Method: Twenty five rats per sex per group were administered ADO for thirteen weeks in feed at target levels of 5, 25, and 125 mg/kg (nominal). Hematology included hematocrit and hemoglobin levels, erythrocyte count, and total and differential leukocyte counts. Serum chemistry included fasting glucose, BUN, total protein, total bilirubin, SGPT, SGOT, alkaline phosphatase, albumin, sodium, potassium, chloride, calcium and carbon dioxide. Urinalysis included specific gravity, pH, ketones, total protein, bilirubin and a miscropic examination of sediment. The following tissues were collected from all rats and examined from the control and high dose groups in 10% neutral buffered formalin: brain, thoracic spinal cord, pituitary, thyroids, adrenals, heart, lungs, spleen, liver, kidneys, stomach, small and large intestines, pancreas, urinary bladder, testes with epididymides and prostate or ovaries and uterus, salivary glands, mesenteric lymph nodes, eyes, nerve with muscle, bone marrow, rib junction and any unusual lesions. Organ weights were measured for the following organs and organ body weight rations were calculated: liver, spleen, heart, testes with epididymides, thyroids and adrenals.
Attained dose: 118.5, 23.8, 4.8 mg/kg (males)
120.2, 24.3, 4.8 mg/kg (females)
Result: No mortality occurred in the study. ADO caused a depression in body weight gain in high-dose females from weeks 3 through 13 of the study. This was associated with a decrease in food consumption. No other signs of toxicity including mortality, clinical signs, changes in hematology or organ weights or gross or microscopic pathology were associated with ADO administration. The N(L)OEL was established assuming that the depression of body weights in females at the highest dose level was a result of reduced food consumption and not a direct toxic effect of ADO.
Reliability: (1) valid without restriction
19-OCT-2005 (19)

Type: Sub-acute
Species: rat **Sex:** male/female
Strain: other: Harlan-Wistar
Route of administration: oral feed
Exposure period: 7 days
Frequency of treatment: continuous
Doses: 250, 500, 1000 mg/kg (study 1); 31.25, 62.5, 125 mg/kg (study 2)
Control Group: yes
NOAEL: = 27.6 mg/kg
LOAEL: = 57.9 mg/kg

Method: other
GLP: no
Test substance: no data

Method: Five rats per group per sex were administered ADO in diet at daily target doses ranging from 31.25 to 1000 mg/kg for 7 days (nominal). Attained dose: 728, 409, 243, 121, 57.9 and 27.6 mg/kg.
Remark: The report describes two separate studies. The initial study was conducted at the higher dose levels followed by a second study at lower dose levels. Parameters examined included mortality, food consumption, bodyweights, and liver and kidney weights.
Result: Lower body weight gains than controls at dose levels at or above 57.9 mg/kg for males and 121 mg/kg for females were observed. The degree of the effect on body weight gains was dose-related, being only slight and transient at the lower dose levels. Food consumption was reduced at the higher dose levels. No deaths occurred. Weights (relative to body weight) of the liver and kidneys were not significantly affected.
Reliability: (2) valid with restrictions
23-SEP-2005 (15)

5.5 Genetic Toxicity 'in Vitro'

Type: Ames test
System of testing: Salmonella typhimurium strains TA98, TA100, TA1535, TA1537 and TA1538
Concentration: 100, 333, 1,000, 3,333, and 10,000 mg/plate
Cytotoxic Concentration: no data
Metabolic activation: with and without
Result: negative

Method: other
GLP: yes
Test substance: no data

Method: Plate incorporation method was used. A solvent control (DMSO) and positive controls were included. The positive controls for tests without metabolic activitation were 2-nitrofluorene (TA98 & TA 1538), sodium azide (TA-100 & TA 1535) and 9-aminoacridine (TA 1537). With activitation, 2-aminoanthracene was used for all strains.The concentrations were
tested in triplicate. Doses were selected from a range finding study. Metabolic activation was obtained from Arochlor-

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induced rat (F-344) and hamsters (Syrian golden).
Reliability: (1) valid without restriction
23-SEP-2005 (22)

Type: Ames test
System of testing: Salmonella typhimurium strains TA98, TA100, TA1535 and TA1538
Concentration: 5, 10, 50, 100, 500, 1,000 and 5,000 mg/plate
Cytotoxic Concentration: 5000 mg/plate
Metabolic activation: with and without
Result: negative

Method: other
GLP: no
Test substance: no data presumed to be >95% based on analyses of other Allied samples.

Method: Plate incorporation method was used. No replicate performed. Concurrent positive control was reported. Metabolic activation used was obtained from Arochlor induced rats.
Reliability: (2) valid with restrictions
19-OCT-2005 (23)

Type: Mouse lymphoma assay
System of testing: L5178Y tk+/- 3.7.2C mouse lymphoma cells
Concentration: 1.1, 1.2, 1.3, 1.4, 1.5,and 1.6 microlitre/mL
Cytotoxic Concentration: 1.6 microlitre/mL
Metabolic activation: with and without
Result: ambiguous

Method: other
GLP: yes
Test substance: no data

Method: Method of Clive and Spector. Doses selected from range finding study. Solvent and positive controls utilized. The solvent was DMSO and the positive controls were ethyl methanesulfonate (w/o activation) and 3-methylcholanthrene (w activation).Study run in duplicate. Metabolic activation was obtained from Aroclor induced F344 rats.
Result: Equivocal result without metabolic activation. A greater than 2-fold increase in mutant frequency was noted only at the highest dose of 1.6 mL/mL which produced only 11% total growth. There was no clear dose-response with the curve being relatively flat. ADO was not mutagenic with metabolic activation.
Reliability: (1) valid without restriction
23-SEP-2005 (22)

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5.6 Genetic Toxicity 'in Vivo'

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5.7 Carcinogenicity

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5.8.1 Toxicity to Fertility

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5.8.2 Developmental Toxicity/Teratogenicity

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Type: other: one-generation reproduciton study
In Vitro/in vivo: In vivo
Species: rat
Strain: other: Wistar outbred(Crl:(WI)WU **Sex:** male/female BR)
Route of administration: gavage
Exposure period: at least 10 weeks (premating, mating, gestation and lactation period).
Frequency of treatment: daily
Doses: 5, 25 and 75 mg/kg bw
Control Group: yes
Result: Decreased number of live born pups, increased number of stillborn pups observed in the high dose groups are the basis for the LOAEL of 25 mg/kg bw and the NOAEL 5 mg/kg bw.

Method: other: OECD 415 and 416
Year: 2005
GLP: yes
Test substance: purity: 98.6-98.8%
Result: Except or decreased activity and/or sedation of the high dose animals, no treatment related clinical findings were observed.
Statistically significant decrease in food consumption in high dose animals and mid dose females during the first week of the study was considered to be related to the administration of the test substance.
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An increase, not statistically significant, in the number of litters with stillborn pups was observed in the high dose group. This effect was considered treatment related.
No other effects were observed on litter size, number of stillborn-, missing- and dead pups during lactation period and on the sex ratio, pup abnormalities or pup weight during lactation. Macroscopic observations, absolute or relative organ weights (brain, spleen and thymus) did not reveal treatment related findings.
Effects on red blood cell variables and on total white blood cell parameters were observed in high dose group animals.
Gross examination of the parental animals at necropsy did not reveal any treatment-related effect.
Microscopic examination of the organs and tissues of parental animals revealed treatment-related histopathological changes in spleen (high dose group animals) and liver (low-, mid- and high dose females and high-dose males).
Reliability: (1) valid without restriction (25)

5.8.3 Toxicity to Reproduction, Other Studies

Type: other: sub-chronic reproduction study
In Vitro/in vivo: In vivo
Species: rat

Strain: Crj: CD(SD) **Sex:** male/female
Route of administration: oral feed
Exposure period: 13 weeks
Frequency of treatment: continuous
Duration of test: 13 weeks
Doses: 5, 25, 125 mg/kg (nominal) Attained dose:
118.5, 23.8, 4.8 mg/kg (males)
120.2, 24.3, 4.8 mg/kg (females)

Control Group: yes
Result: No changes in testicular weight or microscopic pathology of the testes or ovaries were observed.

Method: other
GLP: no
Test substance: no data presumed to be >95% based on analysis of other Allied samples.

Remark: Well designed subchronic study. Criteria evaluated included testes weight and gross and microscopic pathology of the testes and ovaries).
Reliability: (2) valid with restrictions
19-OCT-2005 (19)

Type: other: one-generation reproduciton study
In Vitro/in vivo: In vivo
Species: rat
Strain: other: Wistar outbred(Crl:(WI)WU BR) **Sex:** male/female
Route of administration: gavage
Exposure period: at least 10 weeks (premating, mating, gestation and lactation period).
Frequency of treatment: daily
Doses: 5, 25 and 75 mg/kg bw
Control Group: yes
Result: Decreased number of live born pups, increased number of stillborn pups observed in the high dose groups are the basis for the LOAEL of 25 mg/kg bw and the NOAEL 5 mg/kg bw.

Method: other: OECD 415 and 416
Year: 2005
GLP: yes
Test substance: other TS Purity: 98.6-98.8 %

Result: Except or decreased activity and/or sedation of the high dose animals, no treatment related clinical findings were observed.
Statistically significant decrease in food consumption in high dose animals and mid dose females during the first week of the study was considered to be related to the administration of the test substance.
Fertility or reproductive performance of the male and female animals and the estrus cycle of the females was not affected.
An increase, not statistically significant, in the number of litters with stillborn pups was observed in the high dose groups. This effect was considered treatment related.
No other effects were observed on litter size, number of stillborn-, missing- and dead pups during lactation period and on the sex ratio, pup abnormalities or pup weight during lactation. Macroscopic observations, absolute or relative organ weights (brain, spleen and thymus) did not reveal treatment related findings.
Effects on red blood cell variables and on total white blood cell parameters were observed in high dose group animals.
Gross examination of the parental animals at necropsy did not reveal any treatment-related effect.
Microscopic examination of the organs and tissues of parental animals revealed treatment-related histopathological changes in spleen (high dose group animals) and liver (low-, mid- and high dose females and high-dose males).
Reliability: (1) valid without restriction
27-OCT-2005 (25)

23-SEP-2005

5.9 Specific Investigations

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5.10 Exposure Experience

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5.11 Additional Remarks

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6.1 Analytical Methods

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6.2 Detection and Identification

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7.1 Function

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7.2 Effects on Organisms to be Controlled

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7.3 Organisms to be Protected

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7.4 User

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7.5 Resistance

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8.1 Methods Handling and Storing

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8.2 Fire Guidance

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8.3 Emergency Measures

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8.4 Possib. of Rendering Subst. Harmless

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8.5 Waste Management

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8.6 Side-effects Detection

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8.7 Substance Registered as Dangerous for Ground Water

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8.8 Reactivity Towards Container Material

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10.1 End Point Summary

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10.2 Hazard Summary

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10.3 Risk Assessment

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