OPPT-2003-0063-0075

12 pp

STRUCTURE ACTIVITY TEAM REPORT ver. 04/98

CBI?

Case #:	P-01-0764	**DCN:**	
SAT Date:	8/7/01	**SAT Chair:**	L. Keifer

Submitter: Itochu Specialty Chemicals

Chemical Name:

CAS RN: 39290-90-9	**Trade Name:**

RECEIVED OPPT NCIC 2004 AUG 27 AM 10:54

EPA SANITIZED

Molecular Formula:	$K_2MgO_6Ti_2$		
Molecular Wt. 1000000	**WT%<500:**	**WT%<1000:**	
MP: 1350.00 - 1400.00	**BP:**	**Eq. Wt:**	
H2O Sol (g/L):	<0.000001 ☒	**V.P.**	<0.000001
Max. Prod. Volume (kg/yr):		**Physical State:**	Solid
USE:			

Related Case Numbers	Case Role	Related Case Numbers	Case Role

Focus **Date:** 8-13-01 **Results:** 5 e cat Health, XB-H

STRUCTURE ACTIVITY TEAM REPORT 08/07/01

CASE NUMBER: **P01-0764**

RELATED CASES:

CONCLUSIONS/DISCUSSIONS

TYPE OF CONCERN:	HEALTH	ECOTOX
LEVEL OF CONCERN:	1-2	1

KEYWORDS: LUNG OVERLOAD
ONCO

SUMMARY OF ASSESSMENT

FATE: Solid
S (mg/L, 25°C) < 0.001(E); H < 1.00E-8(E)
MP (C) = 1350-1400(M); BP (C) > 400(E); VP @ 25C (mm) < 1.0E-6(E)
POTW removal (%) = 90 via sorption
Time for complete ultimate aerobic biodeg > mo
PBT Potential: P3B1T1
Sorption to soils/sediments = v.strong
*CEB FATE: Migration to ground water = negl

HEALTH: Absorption is nil all routes (pchem). Concern for lung toxicity if inhaled based on lung overload for poorly soluble particulates; oncogenicity based on lung overload for titanium dioxide.

*CEB HEALTH: Low moderate concern (Inhalation); **Need to know particle size distribution**

Test data: (-) Salmonella with and without activation; (-) E. coli with and without activation; (-) for chromosome aberrations in human lymphocytes with and without activation; rat oral LD_0 = 2000 mg/kg; mouse oral LD_0 = 5000 mg/kg; rat dermal LD_0 = 2000 mg/kg; slight eye irritation in rabbits, cleared by 72 hours; very slight skin irritation in rabbits, cleared by 24 hours; no skin sensitization in guinea pigs using the Magnusson-Kligman assay; rat inhalation LC_{50}>5.04 g/m^3

ECOTOX: Predicted (P) toxicity values in mg/L (ppm) are:

fish 96-h LC50	=	*	P	
daphnid 48-h LC50	=	*	P	
green algal 96-h EC50	=	*	P	
fish Chronic Value (ChV)	=	*	P	
daphnid ChV	=	*	P	
algal ChV	=	*	P	

based on SARs for titanium compounds; SAR chemical class = titanium;

hardness <180.0 mg/L as $CaCO_3$, 100% active ingredients, nominal concentrations, and TOC <2.0 mg/L;
low concern;

assessment factor	=	10.0	
concern concentration (CC)	=	*	mg/L

*CEB ECOTOX: No releases to water

SAT Co-chair: Leonard Keifer 260-1548

B

BIOLOGICAL TEST INFORMATION

Case Number: **P-01-0764** Date Received: **7/25/01** Rev. Init: **CAA** OECD Status: **Incomplete** Page: 1 of 7

Genotoxicity data for: [X] Submitted Substance [] Analog:

[X]AMES	POS/NEG	(with/without activation)	STRAIN IF (+)	
[X]E. coli reverse mutation	POS/NEG	(with/without activation)	[]Mouse Micronucleus	POS/NEG ip/oral
[X]Chromosome Abs in: CHO/CHL	POS/NEG	(with/without activation)	[]Rat Hepatocyte UDS	POS/NEG

Comments: **The chromosome aberration test was performed in human lymphocytes (p. 96)**

Other Data: [X]Ecotox [X]Fate **activated sludge, p200** [X]Water solubility/Log P **<3.6 x 10^-5 g/L @ 20 ± 0.5C, p14** %ai

This information is for: [X] Submitted Substance [] Analog:

Study Type: **Acute Oral**	Study duration:	**15 days**	Species: **Rat**	Sex: **MF**	
Wt/Life stage: **223-429 g/11 wks**	No. groups/No. per group	**1/6**	Controls:		
Route: **Gavage**	Dose range:	**2000 mg/kg**			

Characteristics of tested substance: **white powder, in 1% aqueous carboxymethylcellulose**

Test Conditions (Dosing Regimen): **Animals received a single oral gavage dose of the test substance**

Results: **There were no deaths or clinical signs. Body weight gain was considered normal. At necropsy, reduced testes size was observed in 1 male. The oral LD50 was considered to be greater than 2000 mg/kg.**

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BIOLOGICAL TEST INFORMATION

Case Number: **P-01-0764**	Date Received: **7/25/01**	Rev. Init: **CAA**	OECD Status: **Incomplete**	Page: 2 of 7	
This information is for: [X] Submitted Substance	[] Analog:				
Study Type: **Acute Oral**	Study duration:	**15 days**	Species: **Mice**	Sex: **M**	
Wt/Life stage: **27.6-29.2 g/5 wks**	No. groups/No. per group	**1/5**	Controls: **1/5**		
Route: **Gavage**	Dose range:	**5000 mg/kg**			
Characteristics of tested substance:	**white powder, suspended in corn oil**				
Test Conditions (Dosing Regimen):	**Animals received a single oral gavage dose of the test substance**				
Results:	**There were no deaths or clinical signs in any animal. Body weight gains were considered normal. No abnormalities were detected at necropsy. The oral LD50 in mice was greater than 5000 mg/kg.**				

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BIOLOGICAL TEST INFORMATION

Case Number: **P-01-0764**	Date Received: **7/25/01**	Rev. Init: **CAA**	OECD Status: **Incomplete**	Page: 3 of 7	
This information is for: [X] Submitted Substance	[] Analog:				
Study Type: **Acute Dermal**	Study duration:	**15 days**	Species: **Rat**	Sex: **F**	
Wt/Life stage: **219.5-242.7 g/6 wks**	No. groups/No. per group	**1/5**	Controls: **1/5**		
Route: **Dermal**	Dose range:	**2000 mg/kg**			
Characteristics of tested substance:	**white powder, suspended in corn oil**				
Test Conditions (Dosing Regimen):	**The substance was applied to the clipped skin of each animal and held in place with surgical tape covered with elastic tape. Following a 24-hr exposure, dressings were removed and warm water was used to wash away any residual test substance.**				
Results:	**There were no deaths and no clinical signs noted in any animals throughout the study. Changes in body weight were considered normal. No abnormalities were noted at necropsy. The dermal LD50 was considered greater than 2000 mg/kg in female rats.**				

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BIOLOGICAL TEST INFORMATION

Case Number: **P-01-0764**	Date Received: **7/25/01**	Rev. Init: **CAA**	OECD Status: **Incomplete**	Page: 4 of 7	
This information is for: [X] Submitted Substance	[] Analog:				
Study Type: **Eye Irritation**	Study duration:	**72 hours**	Species: **Rabbit**	Sex: **M**	
Wt/Life stage: **1-3.5 kg/6 wks**	No. groups/No. per group	**1/3**	Controls:		
Route: **Ocular**	Dose range:	**84 mg (0.1 ml)**			
Characteristics of tested substance:	**white powder**				
Test Conditions (Dosing Regimen):	**The test substance was instilled into the conjunctival sac of 1 eye of each animal.**				
Results:	**Irritation of the conjunctivae (redness, chemosis, discharge) was seen, but had completely resolved within 72 hours in 2 animals and within 48 hours in the other animal. Iridial irritation (grade 1) was observed on day 1 and resolved within 24 hours. Remnants of the test substance were present in the eyes of all animals on day one.**				

BIOLOGICAL TEST INFORMATION

Case Number: **P-01-0764**	Date Received: **7/25/01**	Rev. Init: **CAA**	OECD Status: **Incomplete**	Page: 5 of 7	
This information is for: [X] Submitted Substance	[] Analog:				
Study Type: **Skin Irritation**	Study duration:	**72 hours**	Species: **Rabbit**	Sex: **M**	
Wt/Life stage: **1845-2342 g/8-13 wks**	No. groups/No. per group	**1/3**	Controls:		
Route: **Dermal**	Dose range:	**0.5 g**			
Characteristics of tested substance:	**white powder**				
Test Conditions (Dosing Regimen):	**The test substance was applied to the clipped skin of each animal and secured for 4 hours with a semi-occlusive wrap. After exposure, the skin was cleaned of residual test material with water.**				
Results:	**Very slight erythema was seen at the treated sites of all animals, and had resolved within 24 hours.**				

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BIOLOGICAL TEST INFORMATION

Case Number: **P-01-0764**	Date Received: **7/25/01**	Rev. Init: **CAA**	OECD Status: **Incomplete**	Page: 6 of 7	
This information is for: [X] Submitted Substance	[] Analog:				
Study Type: **Skin Sensitization**	Study duration:	**1 month**	Species: **Guinea Pig**	Sex: **F**	
Wt/Life stage: **281-399 g/NS**	No. groups/No. per group	**1/10**	Controls: **1/5**		
Route: **Intradermal, dermal**	Dose range:	**intradermal injection:10% concentration in water; dermal:50% concentration in 1% aqueous carboxymethylcellulose; challenge:50% concentration in 1% aqueous carboxymethylcellulose**			
Characteristics of tested substance: **white powder**					
Test Conditions (Dosing Regimen): **The method described by Magnusson and Kligman was used.**					
Results: **No skin reactions were evident following the challenge exposure. There was no evidence that the substance caused sensitization in the guinea pig.**					

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BIOLOGICAL TEST INFORMATION

Case Number: **P-01-0764**	Date Received: **7/25/01**	Rev. Init: **CAA**	OECD Status: **Incomplete**	Page: 7 of 7	
This information is for: [X] Submitted Substance	[] Analog:				
Study Type: **Acute Inhalation**	Study duration:	**15 days**	Species: **Rat**	Sex: **MF**	
Wt/Life stage: **approx. 199-320 g/NS**	No. groups/No. per group	**1/10**	Controls:		
Route: **nose-only inhalation**	Dose range:	**5.04±0.17g/m3**			
Characteristics of tested substance: **white powder**					
Test Conditions (Dosing Regimen): **Animals were exposed to the test substance via nose-only inhalation for 4 hours.**					
Results: **A slightly decreased breathing rate was seen in all animals at all observation times. In 1 male and 2 female rats, slight labored breathing was seen in the last 1-2 hours of exposure. The inhalation 4-hr LC50 was greater than 5.04±0.17g/m3.**					

NCSAB SAT REPORT		CBI? (Y/N):
PMN: P-01-0764	CAS RN:	39290-90
Chemical Name: Magnesium potassium titanium oxide		Analogs:
		Production Volume:

Structure:

Formula:	$K_2MgO_6Ti_2$		Eq Wt:		
Mol Weight:	∞ ~~294.31~~	Wt%<500:		Wt%<1000	
MP:	1350.00 - 1400.00		BP:		VP: <0.000001
H2O Sol (g/L):	<0.000001	Physical State:	Solid	Log P:	

Endpoint (mg/L)	Est. Value	Meas. Value	Comments
Fish 96-h	*		
Daphnid 48-h	*		
Algal 96-h	*		
Fish ChV	*		
Daphnid ChV	*		
Algal ChV	*		
BCF			

CHEMICAL CLASS:				SAR: Ti	
ECOTOX CONCERN	H	M	L	CONCERN CONCENTRATION	*
DATE 8/7/01				ASSESSOR:	

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OPPT STRUCTURE ACTIVITY TEAM (SAT) MEETING DATE 8-7-01

ATTENDEES	SIGNATURE
CHEMISTRY	
✓ Paul Bickart	
Diana Darling	
✓ Rich Engler	
Greg Fritz	
Daniel Lin	
✓ Kathy Schechter	Kathy Schechter
ENVIRONMENTAL FATE	
Bob Boethling	
David Lynch	
Gary Thom	
HEALTH	
Katherine Anitole	
✓ Michael Cimino	
Leonard Keifer	
David Lai	
Jim Murphy	
Deborah Norris	
Ronald Ward	
✓ Yin Tak Woo	
ENVIRONMENTAL EFFECTS	
Gordon Cash	
Vince Nabholz	
✓ Maggie Wilson	Maggie Wilson
SAT CHAIRPERSON/OTHER	
Rebecca Jones	
✓ Leonard Keifer	
Vince Nabholz	