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INITIAL SUBMISSION: MATERIAL SAFETY DATA SHEET ON SANTOCURE VULCANIZATION ACCELERATOR WITH COVER LETTER DATED 01/11/84		
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SANTOCURE VULCANIZATION ACCELERATOR		

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Monsanto

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January 11, 1984

12-414 B

Mr. Martin Greif
Executive Secretary
TSCA Interagency Testing Committee
Environmental Protection Agency (TS-792)
401 "M" Street, SW
Washington, DC 20460

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RECEIVED
OPPT CBIC

Dear Sir:

This letter is in response to the ITC listing of N-cyclohexyl-2-benzothiazolesulfenamide, CAS #95-33-0, in the Federal Register of Wednesday, November 9, 1983, page 51520. Monsanto manufactures this chemical under the trade name SANTOCURE® vulcanization accelerator. The chemical is also called CBS and will so be referred to in the following statements.

Acute toxicologic effects have been investigated by Monsanto, and have found to be relatively minor. Specifically, the oral LD₅₀ (Rats) is 5,300 mg/kg, or Practically Nontoxic. The acute dermal LD₅₀ (Rabbit) is greater than 7940 mg/kg, or Practically Nontoxic. Acute eye irritation (Rabbit) for CBS is 1.8 on a scale of 110.0 (FHSA), Practically Non-irritating, and the acute skin irritation (Rabbit) is 0.0 on a scale of 8.0 (FHSA), Practically Non-irritating.

Patch testing of 51 human volunteers with CBS in a 70% preparation in petrolatum produced sensitization in 5 of 51 subjects. No evidence of primary or cumulative irritation was observed. This chemical was considered to be a potential skin sensitizer.

In a four week dust inhalation study, rats were exposed to CBS at average concentrations of 4.3, 14.4 and 48.0 mg/m³, six hours/day, five days/week. Elevated clinical chemistry (SGOT) values were observed in mid and high dose animals. The significance of this finding is unclear. Microscopic lesions in the conjunctiva lymph nodes and spleen were noted for high exposure group animals at an incidence greater than control animals. The highest no-effect level in this study is 14.4 mg/m³.

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Mr. Martin Greif

- 2 -

January 11, 1984

In a four week dietary range study, rats were fed diets containing CBS at dosage levels of 0, 100, 250, 1000 or 3000 mg/kg of body weight. Evidence of toxicity, as indicated by reduced body weight gains in food consumption was noted at 500, 1000 and 3000 mg/kg dosage levels. Maximum dosage producing no significant effect on test animals was 250 mg/kg of CBS.

Repeated dermal application of CBS to the intact and abraded skin of rabbits of 125, 500 or 200 mg/kg for 21 days produced no evidence of toxicity related to test material application.

No teratogenic effects were observed on groups of 25 mated female rabbits when treated orally with CBS at dosages of 100, 300 or 500 mg/kg of body weight on day 6 through 15 of gestation. Fetal body weight means and maternal body weight gains were significantly reduced in the 500 mg/kg dosage group. No adverse maternal or fetal effects were observed upon administration of CBS up to 300 mg/kg.

CBS is used as a rubber vulcanization accelerator for the production of vehicle tires. The compound is chemically altered during the vulcanization process, and is bound up in the rubber matrix.

CBS is used primarily by sophisticated manufacturers who recognize the need for employee personal protective devices and processes designed to protect workers. The cost of CBS is sufficiently high to motivate manufacturers to avoid spills and conserve material for process use as much as possible.

To illustrate the extent to which rubber chemical manufacturers are informing workers about safety and handling of CBS, enclosed is a Monsanto Material Safety Data Sheet covering this product.

Monsanto will be pleased to provide you with copies of toxicologic test results upon request.

Sincerely,

Bernard J. Hill (ms)

Bernard J. Hill
Product Acceptability Manager
Rubber Chemicals

Enclosure

15.1005/SS.2

Monsanto MATERIAL SAFETY DATA

1R-414B

Page 1 of 4

MONSANTO PRODUCT NAME
**SANTOCURE® VULCANIZATION
ACCELERATOR**

MONSANTO COMPANY
800 N. LINDBERGH BLVD.
ST. LOUIS, MO 63167

Emergency Phone No.
(Call Collect)
314-694-1000

PRODUCT IDENTIFICATION

Synonyms:	N-cyclohexyl-2-benzothiazolesulfenamido; 2-benzothiazole sulfenamido, N-cyclohexyl
CAS No.:	95-33-0
DOT Proper Shipping Name:	Not Applicable
DOT Hazard Class/ I.D. No.:	Not Applicable
DOT Label:	Not Applicable
Hazardous Substance(s)/ RQ(s):	Not Applicable
U.S. Surface Freight Classification:	Rubber Accelerator, N.O.I.B.N.

WARNING STATEMENTS

WARNING!
MAY CAUSE ALLERGIC SKIN REACTION
MAY LIBERATE IRRITATING FREE AMINE

PRECAUTIONARY MEASURES

Avoid prolonged or repeated contact with skin.
Avoid prolonged or repeated inhalation of vapor.
Wash thoroughly after handling.

STORE IN COOL, WELL VENTILATED PLACE AWAY FROM FOODSTUFFS AND ACIDS.

EMERGENCY AND FIRST AID PROCEDURES

FIRST AID: IF IN EYES, flush with water. Remove contaminated clothing. Wash clothing before reuse.

IF ON SKIN, immediately wash with soap and plenty of water.

OCCUPATIONAL CONTROL PROCEDURES

Eye Protection: SANTOCURE® vulcanization accelerator does not present significant eye irritation or eye toxicity requiring special protection.

Skin Protection: Wear appropriate impervious gloves and protective clothing to prevent skin contact. Wear face shields and aprons when splashing is likely. Launder contaminated clothing before re-use. Attention! Repeated or prolonged contact may cause allergic skin reaction in some people.

(Occupational Control Procedures Continued On Next Page)

MATERIAL SAFETY DATA

Santocure® Vulcanization Accelerator

OCCUPATIONAL CONTROL PROCEDURES (Continued)

Respiratory Protection: Use NIOSH approved equipment when airborne exposure is excessive. Consult respirator manufacturer to determine appropriate type equipment for given application.

Ventilation: Provide ventilation to minimize exposure. Local exhaust ventilation preferred.

Airborne Exposure Limits: Product: N-cyclohexyl-2-benzothiazolesulfenamide Wt. % 96
 Although no specific exposure limit has been established for this material, OSHA and ACGIH have established limits for nuisance dusts:
 OSHA PEL/TWA: Total 15 mg/m³; Respirable 5 mg/m³
 ACGIH TLV/TWA: Total 10 mg/m³; Respirable 5 mg/m³
 These limits are stated only to indicate the least stringent airborne dust exposure levels applicable to nuisance dusts. Santocure may cause sensitization at exposure concentrations below these limits.

FIRE PROTECTION INFORMATION

Combustible Solid

Flash Point: 350°F (Liquified Material) **Method:** Cleveland Open Cup

Ignition Temperature: 660°F (Dust Cloud)

Extinguishing Media: Water or any Class A extinguishing agent.

Special Firefighting Procedures: When exposed to products of combustion firefighters should wear self-contained breathing apparatus and full protective clothing including boots. When burned, SANTOCURE may liberate toxic carbon monoxide, sulfur dioxide, nitrogen oxides, fumes and tertiary butyl amine.

Unusual Fire And Explosion Hazards: Powder or dust will form explosive concentrations when mixed in sufficient quantities in air.

REACTIVITY DATA

Thermally stable.

Materials to Avoid: Avoid storage near foodstuffs and acids.

Hazardous Decomposition Products: Carbon monoxide, nitrogen oxides and sulfur dioxide fumes are liberated when product is ignited. Cyclohexylamine vapor may be emitted during processing conditions or a fire.

Hazardous Polymerization: Does not occur.

PHYSIOLOGICAL EFFECTS SUMMARY

Oral LD₅₀ (Rat): 5,300 mg/kg, Practically Nontoxic
 Dermal LD₅₀ (Rabbit): >7,940 mg/kg, Practically Nontoxic
 Eye Irritation (Rabbit): (FHSA) 1.8 on a scale of 110.0, Slightly Irritating
 Skin Irritation (Rabbit): (FHSA) 0.0 on a scale of 8.0, Practically Nonirritating
 (Physiological Effects Summary Continued On Next Page)

Santocure® Vulcanization Accelerator

MATERIAL SAFETY DATA



PHYSIOLOGICAL EFFECTS SUMMARY (Continued)

The following information represents the results of experiments conducted to assess the physiological properties of this material. This information was used by qualified experts to develop the Warning Statements and the recommended Occupational Control Procedures. Because dosages were intentionally chosen to induce toxic effects, evaluation of the significance of the data from individual studies may require professional knowledge of toxicology. Extensive evaluation of the available information indicates that SANTOCURE vulcanization accelerator can be handled safely if the recommended procedures are followed.

During storage or use, breakdown of SANTOCURE may occur causing release of: mercaptobenzothiazole, a known sensitizer; and cyclohexylamine which at sufficient concentration, may cause respiratory or dermal irritation.

Patch testing of 51 human volunteers with SANTOCURE as a 70% preparation in petrolatum produced sensitization in 5 of 51 subjects. No evidence of primary or cumulative irritation was observed. This chemical was considered to be a potential skin sensitizer.

In a 4-week dust inhalation study, rats were exposed to SANTOCURE at average concentrations of 4.3, 14.4 and 48.0 mg/m³, 6 hours/day, 5 days/week. Elevated clinical chemistry (SGOT) values were observed in mid and high dose animals. The significance of this finding is unclear. Microscopic lesions in the conjunctiva, lymph nodes and spleen were noted for high exposure group animals at an incidence greater than control animals. The highest no-effect level in this study is 14.4 mg/m³.

In a 4-week dietary range study, rats were fed diets containing SANTOCURE vulcanization accelerator at dosage levels of 0, 100, 250, 1000 or 3000 mg/kg of body weight. Evidence of toxicity, as indicated by reduced body weight gains and food consumption was noted at 500, 1000 and 3000 mg/kg dosage levels. The maximum dosage producing no significant effect on test animals was 250 mg/kg SANTOCURE.

Repeated dermal application of SANTOCURE to the intact and abraded skin of rabbits at dosages of 125, 500 or 2000 mg/kg for 21 days produced no evidence of toxicity related to test material application.

No teratogenic effects were observed when groups of 25 mated female rabbits were treated orally with SANTOCURE at dosages of 100, 300 or 500 mg/kg of body weight on days 6 through 15 of gestation. Fetal body weight means and maternal body weight gains were significantly reduced in the 500 mg/kg dosage group. No adverse maternal or fetal effects were observed upon administration of SANTOCURE up to 300 mg/kg.

PHYSICAL DATA

Appearance:	Light tan to buff powder or pellets
Odor:	Slight amine
Melting Point:	197°C
Specific Gravity @ 25°C/4°C:	1.27 - 1.3
Solubility in Water:	Insoluble
in Benzene:	Soluble
in Acetone:	Soluble
in Hexane:	1.7 g/100 ml
in Ethyl Ether:	Soluble
in Alcohol:	Moderately soluble

Note: These physical data are typical values based on material tested but may vary from sample to sample. Typical values should not be construed as a guaranteed analysis of any specific lot or as specification items.

SPILL, LEAK & DISPOSAL INFORMATION

Waste Disposal: Dispose of in a chemical landfill which complies with all local, state and federal regulations.

Spill or Leakage Procedures: Vacuum or sweep up and place in dry, covered container. Flush area with water.

Container: Dispose of in a chemical landfill which complies with all local, state and federal regulations.

ADDITIONAL COMMENTS

SANTOCURE vulcanization accelerator slowly degrades on storage particularly under warm, humid conditions. Keep stocks below 40°C, dry and away from sunlight. Keep containers closed. Store away from insoluble sulfur as traces of amines can cause reversion to soluble sulfur.

For further information on sulfenamide storage and handling, consult the Rubber Chemicals Division publication "Rubber Chemicals Stability."

Environmental Toxicity Information:

- 96-hr LC₅₀ Rainbow Trout: 5.4 mg/l, Mildly Toxic
- 96-hr LC₅₀ Bluegill: 7.9 mg/l, Mildly Toxic
- 96-hr LC₅₀ Algae Cell Count: 1.1 mg/l, Moderately Toxic
Chlorophyll α : 0.9 mg/l, Highly Toxic
- 96-hr LC₅₀ Fathead Minnow: >1,000 mg/l, Practically Nontoxic
- 48-hr LC₅₀ *Daphnia*: 18 mg/l, Slightly Toxic

DATE: 10/06/83 **REVISED:** X **SUPERSEDES:** 12/18/80
MSDS NO.: 000095330

FOR ADDITIONAL NON-EMERGENCY INFORMATION, CONTACT:

Manager, Product Acceptability
 Monsanto Polymer Products Company
 Rubber Chemicals Division
 314-694-1000

Although the information and recommendations set forth herein (hereinafter "information") are presented in good faith and believed to be correct as of the date hereof, Monsanto Company makes no representations as to the completeness or accuracy thereof. Information is supplied upon the condition that the persons receiving same will make their own determination as to its suitability for their purposes prior to use. In no event will Monsanto Company be responsible for damages of any nature whatsoever resulting from the use of or reliance upon information. NO REPRESENTATIONS OR WARRANTIES, EITHER EXPRESS OR IMPLIED, OF MERCHANTABILITY, FITNESS FOR A PARTICULAR PURPOSE OR OF ANY OTHER NATURE ARE MADE HEREUNDER WITH RESPECT TO INFORMATION OR THE PRODUCT TO WHICH INFORMATION REFERS.

This form has been approved by the Occupational Safety and Health Administration as "equivalent to" OSHA Form 20.

Santocure® is a registered trademark of Monsanto Company.

MATERIAL SAFETY DATA Santocure® Vulcanization Accelerator

MONSANTO PRODUCT NAME

SANTOCURE[®]
VULCANIZATION ACCELERATOR

MONSANTO COMPANY
800 N. LINDBERGH BLVD.
ST. LOUIS, MO 63167
EMERGENCY PHONE NO.
(CALL COLLECT)
314-694-1000

PRODUCT IDENTIFICATION

Common Names: CBS, CBTS

Chemical Name: N-cyclohexyl-2-benzothiazolesulfenamide; 2-benzothiazole sulfenamide, N-cyclohexyl-; CBS

CAS No.: 95-33-0

DOT Proper Shipping Name: Not Applicable

DOT Hazard Class/I.D. No.: Not Applicable

DOT Label: Not Applicable

U.S. Surface Freight Classification: Rubber Accelerator, N.O.I.B.N.

Reportable Quantity (RQ) (40 CFR Part 117)

Under Clean Water Act Regulations: Not Applicable

This substance is identified as a hazardous chemical under the criteria of the OSHA Hazard Communications Standard (29 CFR 1910.1200). Substances listed below may be present following storage and/or during processing, and are identified as hazardous chemicals under the criteria of the OSHA Hazard Communication Standard (29 CFR 1910.1200):

mercaptobenzothiazole disulfide, CAS No.: 120-78-5

cyclohexylamine, CAS No.: 108-91-8

2-mercaptobenzothiazole, CAS No.: 149-30-4

benzothiazole, CAS No.: 95-16-9

For specific physical and health hazards or occupational control procedures on these substances, please refer to the appropriate Occupational Control Procedures and Health Effects Summary sections in this Material Safety Data Sheet.

WARNING STATEMENTS

WARNING!

CAUSES IRRITATION TO EYES, SKIN AND RESPIRATORY TRACT
MAY CAUSE ALLERGIC SKIN REACTION

SANTOCUR® VULCANIZATION ACCELERATOR**PRECAUTIONARY MEASURES**

Avoid contact with eyes, skin and clothing.
Avoid breathing dust or vapor.
Wash thoroughly after handling.
Keep container closed.
Use with adequate ventilation.

Emptied container retains vapor and product residue. Observe all labeled safeguards until container is destroyed. **DO NOT REUSE THIS CONTAINER.**

STORE IN A COOL, WELL VENTILATED PLACE AWAY FROM FOODSTUFFS, REDUCING AGENTS AND ACIDS.

EMERGENCY AND FIRST AID PROCEDURES

FIRST AID: IF IN EYES, immediately flush with plenty of water for at least 15 minutes. Call a physician.

IF ON SKIN, immediately wash with soap and plenty of water. Remove contaminated clothing. Wash clothing before reuse.

IF INHALED, remove to fresh air. If not breathing, give artificial respiration, preferably mouth-to-mouth. If breathing is difficult, give oxygen. Call a physician. Remove material from eyes, skin and clothing.

OCCUPATIONAL CONTROL PROCEDURES

Eye Protection: Wear chemical splash goggles to prevent eye contact. Have eye baths available where there is significant potential for eye contact.

Skin Protection: Wear appropriate protective gloves that provide a barrier and protective clothing to prevent skin contact. Consult glove manufacturer to determine appropriate type glove for given application. Wash contaminated skin promptly. Launder contaminated clothing and clean protective equipment before reuse. Wash thoroughly after handling. **ATTENTION!** Repeated or prolonged contact may cause allergic skin reaction on some people.

Respiratory Protection: Avoid breathing dust or vapor of this material. Use NIOSH/MSHA approved equipment when airborne exposure is excessive (see information under "Airborne Exposure Limits" below). Full facepiece equipment is recommended and, if used, replaces need for chemical splash goggles. Consult respirator manufacturer to determine appropriate type equipment for given application. The respirator use limitations specified by NIOSH/MSHA or the manufacturer must be observed. High airborne concentrations may require use of self-contained breathing apparatus or supplied air respirator. Respiratory protection programs must be in compliance with 29 CFR 1910.134.

OCCUPATIONAL CONTROL PROCEDURES (continued)

Ventilation: Provide sufficient ventilation to minimize exposure (see information under "Airborne Exposure Limits" below). Use local mechanical exhaust ventilation at sources of air contamination such as open process equipment. Consult NFPA Standard 91 for design of exhaust system.

Airborne Exposure Limits:

Product: N-cyclohexyl-2-benzothiazolesulfenamide

Although OSHA and ACGIH have not established specific exposure limits for this material, they have established the following limits for nuisance dusts:

OSHA PEL/8-hour Time-weighted average: Total 15 mg/m³; Respirable 5 mg/m³
ACGIH TLV/8-hour Time-weighted average: Total 10 mg/m³; Respirable 5 mg/m³

These limits are stated only to indicate the least stringent airborne dust exposure levels applicable to nuisance dusts. NOTE: SANTOCURE® vulcanization accelerator may cause irritation to eyes, skin and upper respiratory tract and may cause allergic skin reactions and/or sensitization at exposure concentrations below these limits.

Component: Cyclohexylamine

OSHA PEL/8-hour Time-weighted average: None established
ACGIH TLV/8-hour Time-weighted average: 10 ppm (40 mg/m³) - Skin*

* Skin notation means that skin absorption of this material may add to the overall exposure. Avoid skin contact.

Component: Benzothiazole

OSHA PEL/8-hour Time-weighted average: None established
ACGIH TLV/8-hour Time-weighted average: None established

Component: 2-Mercaptobenzothiazole

Although OSHA and ACGIH have not established specific exposure limits for this material, they have established the following limits for nuisance dusts:

OSHA PEL/8-hour Time-weighted average: Total 15 mg/m³; Respirable 5 mg/m³
ACGIH TLV/8-hour Time-weighted average: Total 10 mg/m³; Respirable 5 mg/m³

These limits are stated only to indicate the least stringent airborne dust exposure levels applicable to nuisance dusts. NOTE: Mercaptobenzothiazole may cause allergic skin reactions in some people at exposure concentrations below these limits.

Component: Mercaptobenzothiazole disulfide

The above stated nuisance dust information for 2-mercaptobenzothiazole applies also to mercaptobenzothiazole disulfide. NOTE: This material may cause irritation to skin and respiratory tract and allergic skin reaction at exposure concentrations below the above stated airborne dust exposure limits.

FIRE PROTECTION INFORMATION

Combustible Solid.

Flash Point: ~350°F

Method: Cleveland Open Cup

Melting Point: 216°F

Ignition Temperature: ~660°F (Dust Cloud)

Extinguishing Media: Water spray or any Class A extinguishing agent.

Special Firefighting Procedures: Firefighters and others exposed to products of combustion (see "Hazardous Decomposition Products" below) should wear full protective clothing including self-contained breathing apparatus. Equipment should be thoroughly decontaminated after use.

Unusual Fire and Explosion Hazards: When mixed in sufficient quantities of air a dust explosion can occur. Gaseous products of decomposition may include toxic nitrogen oxides, sulfur dioxide, cyclohexylamine and carbon monoxide.

REACTIVITY DATA

Thermally stable to 218°C.

Materials to Avoid: Avoid storage near reducing agents and acids.

Hazardous Decomposition Products: During long-term storage at extremes of temperature and humidity, or during processing, the following decomposition products may be generated from Santocure vulcanization accelerator:

mercaptobenzothiazole disulfide, CAS No.: 120-78-5
cyclohexylamine, CAS No.: 108-91-8
2-mercaptobenzothiazole, CAS No.: 149-30-4
benzothiazole, CAS No.: 95-16-9

For specific component toxicity information, please refer to the appropriate section in this Material Safety Data Sheet.

Carbon monoxide, nitrogen oxides and sulfur dioxide fumes are liberated when product is ignited. Cyclohexylamine vapor may be emitted during processing conditions or a fire.

Hazardous Polymerization: Does not occur.

HEALTH EFFECTS SUMMARY

The following information presents both human experience and the results of scientific experiments used by qualified experts to assess the effects of SANTOCURE vulcanization accelerator on the health of industrially exposed individuals and to support the Precautionary Measures and Occupational Control Procedures recommended in this document. To avoid misunderstanding, the data provided in this section should be interpreted by individuals trained in evaluation of this type of information.

Data for SANTOCURE vulcanization accelerator**Human Experience**

Dermal contact and inhalation are expected to be the primary routes of occupational exposure to SANTOCURE vulcanization accelerator. Occupational exposure to this material has been reported to cause irritation to the eyes, skin and upper respiratory tract. Allergic skin reactions have been also reported in skin tests with human subjects.

Toxicological Data

Data from Monsanto studies and from the scientific literature indicate the following:

Oral LD₅₀ (Rat): 5,300 mg/kg, Practically Nontoxic
Dermal LD₅₀ (Rabbit): >7,940 mg/kg, Practically Nontoxic
Eye Irritation (Rabbit): (FHSA) 1.8 on a scale of 110.0, Slightly Irritating
Skin Irritation (Rabbit): (FHSA) 0.4 on a scale of 8.0, Practically Nonirritating

Patch testing of 51 human volunteers with SANTOCURE vulcanization accelerator at a 70% preparation in petroleum produced sensitization in 5 of 51 subjects. No evidence of primary or cumulative irritation was observed. This chemical was considered to be a potential skin sensitizer.

In a 4-week dust inhalation study, rats were exposed to SANTOCURE vulcanization accelerator at average concentrations of 4.3, 14.4 and 48.0 mg/m³, 6 hours per day, 5 days per week. Elevated clinical chemistry (SGOT) values were observed in mid and high dose animals. Microscopic lesions in the conjunctiva, lymph nodes and spleen were noted for high exposure group animals at an incidence greater than control animals. The highest no-effect level in this study is 14.4 mg/m³.

In a 4-week dietary range finding study, rats were fed diets containing SANTOCURE vulcanization accelerator at dietary levels equivalent to 0, 100, 250, 1,000 or 3,000 mg/kg of body weight. Evidence of toxicity, as indicated by reduced body weight gains and food consumption was noted at 500, 1,000 and 3,000 mg/kg dosage levels. The maximum dosage producing no significant effect on test animals was 250 mg/kg SANTOCURE vulcanization accelerator.

HEALTH EFFECTS SUMMARY (continued)

N-cyclohexyl-2-benzothiazolesulfenamide (CBS) was evaluated for toxicity in studies in which 2 groups of mice were given either a single subcutaneous injection of the test material at a dosage of 1000 mg/kg followed by observation for 78 weeks, or 215 mg/kg of the test material by oral intubation for 21 days, followed by administration of a diet containing CBS at a dietary concentration equivalent to 90 mg/kg/day for 79 weeks. No adverse effects were reported, and no statistically significant increases in tumor incidences were observed in either study.

Repeated dermal application of SANTOCURE vulcanization accelerator to the intact and abraded skin of rabbits at dosages of 125, 500 or 2000 mg/kg for 21 days produced no evidence of toxicity related to test material application.

No teratogenic effects were observed when groups of 25 mated female rats were treated orally with SANTOCURE vulcanization accelerator at dosages of 100, 300 or 500 mg/kg of body weight on days 6 through 15 of gestation. Fetal body weight means and maternal body weight gains were significantly reduced in the 500 mg/kg dosage group. No adverse maternal or fetal effects were observed upon administration of SANTOCURE vulcanization accelerator up to 300 mg/kg. However, a published study reports an increase in embryonic mortality and a slight decrease in fetal body weights when SANTOCURE vulcanization accelerator was administered orally to a group of 12 to 15 pregnant rats on the fourth and eleventh days of gestation at a dosage of 2000 mg/kg.

SANTOCURE vulcanization accelerator was evaluated in a dominant lethal mutation assay in which 2000 mg/kg of the test material was administered orally to a group of 10 to 11 female rats for 2 days prior to mating or to a group of male rats for 3 days prior to mating. An increase in total embryonic mortality was observed in treated females and in untreated females mated with treated males.

SANTOCURE vulcanization accelerator was evaluated in the L5178TK mouse lymphoma mutation assay and in microbial mutagenicity assays. The microbial assays used five Salmonella strains, with and without microsomal activation, and one Saccharomyces yeast strain. No mutagenic effects were demonstrated in any of these assays.

SANTOCURE vulcanization accelerator was evaluated in a guinea pig sensitization study in which a 25% concentration of the test material (in ethanol) was applied to the shaved skin of the test animals for 6 hours, once a week, for 3 consecutive weeks. A challenge application was administered two weeks after the weekly applications. Under the conditions of this test, SANTOCURE vulcanization accelerator did not cause delayed hypersensitivity in the guinea pig.

In a 4-week comedogenicity (acnegenicity) assay, SANTOCURE vulcanization accelerator was applied daily to the inner surface of rabbit ears 5 days per week at concentrations of 0.01, 0.1 or 10% in chloroform. No production of comedones was observed after repeated treatment with SANTOCURE vulcanization accelerator.

HEALTH EFFECTS SUMMARY (continued)

Additional Information

Stability.

During storage or use, decomposition of SANTOCURE vulcanization accelerator may occur causing release of cyclohexylamine, benzothiazole, 2-mercaptobenzothiazole, and mercaptobenzothiazole disulfide.

Data for cyclohexylamine

Oral LD₅₀ (Rat): >590 mg/kg, Slightly Toxic
Dermal LD₅₀ (Rabbit): 630 mg/kg, Moderately Toxic
Eye Irritation (Rabbit): (FHS) Corrosive
Skin Irritation (Rabbit): (FHS) Corrosive
Vapor Inhalation (Rat): 0 out of 6 rats died when exposed to 13.7 mg/l, nominal concentration in air, of cyclohexylamine for 6 hours. 2 out of the 6 animals were blinded.

Microbial mutagenicity assays using five Salmonella strains with and without mammalian microsomal activation and one yeast strain did not reveal any mutagenic activity.

Groups of rats were administered a diet containing 600, 2,000 or 6,000 ppm cyclohexylamine for 13 weeks. At the two higher dosage levels reduced body weight gain, food intake and relative testis weight in addition to reduced spermatogenesis were observed. The no-effect level for this study was determined to be 600 ppm cyclohexylamine in the diet.

Reduction of testicular spermatogenesis was observed in rats and dogs receiving 200 mg/kg/day and 250 mg/kg/day, respectively by oral gavage for 90 days. The effect was reversible in dogs but not in rats after a 13 week recovery period. A no-effect level was not determined in this study.

No reproductive effects were observed when groups of male rats fed either 0 or 6,000 ppm cyclohexylamine in the diet for 10 months were mated with untreated females. No effects on animal fertility, litter size or offspring were noted.

Data for benzothiazole

Oral LD₅₀ (Rat): 492 mg/kg, Moderately Toxic
Dermal LD₅₀ (Rabbit): >631 mg/kg, Moderately Toxic
Eye Irritation (Rabbit): (AVG. MAX) 61.0 on a scale of 110.0, Severely Irritating
Skin Irritation (Rabbit): (AVG. MAX) 3.0 on a scale of 9.0, Moderately Irritating
Vapor Inhalation (Rat): No mortalities occurred when rats were exposed to benzothiazole at a concentration of 1.4 mg/l in air for 6 hours at 25°C.

Microbial mutagenicity assays using five Salmonella strains and one yeast strain with and without mammalian microsomal activation did not reveal any mutagenic effect.

EFFECTS SUMMARY (continued)

2-mercaptobenzothiazole

(Rat): 3,800 mg/kg, Slightly Toxic
(Rabbit): >7,940 mg/kg, Practically Nontoxic
Irritation (Rabbit): (FHA) 3.2 on a scale of 110.0, Slightly Irritating
Sensitization (Rabbit): (FHA) 0.0 on a scale of 8.0, Nonirritating
LD50 (Rat): >1,270 mg/m³

Irritant patch test on 50 human volunteers with 2-mercaptobenzothiazole showed no positive reactions following the initial application, any of the 15 applications, or subsequent challenge applications made 10-14 days later. Results of these tests, it is concluded that this material is not a primary irritant, a cumulative irritant, or a sensitizing agent. However, sensitization was observed when 2-mercaptobenzothiazole was evaluated in guinea pig sensitization assays.

10 male and 10 female rats and mice were administered 2-mercaptobenzothiazole by gavage at dose levels of 0, 188, 375, 750 and 1,500 mg/kg/day in corn oil for 13 weeks. Male mice showed increased mortality at 1,500 mg/kg/day and female mice had increased mortality at 750 and 1,500 mg/kg/day. Liver weights for both sexes of mice were elevated at 1,500 mg/kg/day, treatment-related histological lesions were noted in the liver. The rats showed no excess mortality, but did show reduced body weights at 375, 750 and 1,500 mg/kg/day. Relative liver weights were significantly increased in all groups of rats of both sexes, but no histopathological lesions of the liver were found.

2-mercaptobenzothiazole was evaluated in a chronic toxicity study using B6C3F1 mice. Animals were administered the test material as daily oral gavage of 100 mg/kg by gavage from 7 to 28 days of age followed by dietary restriction of this dosage for the remainder of the study, or by single intramuscular injection of 215 or 1,000 mg/kg at 28 days of age. All surviving animals were sacrificed at approximately 18 months of age. An increase in the incidence of cell sarcomas at the site of injection was observed in B6C3F1 mice administered 215 mg/kg or daily in the diet. No significant increases were observed in the other strain.

In a study, several strains of mice were given 2-mercaptobenzothiazole at a dosage of 664 mg/kg by subcutaneous injection on days 6 through 15 of gestation. In all strains, increased incidences of fetal malformations were noted but only at the highest toxic doses; this increased incidence was not seen in a repeat study with one of the strains of mice. Administration of 2-mercaptobenzothiazole at a concentration of 200 mg/kg to rats on days 4 and 11 of gestation resulted in increased embryo lethality. In a more complete study, no evidence of teratogenic activity or embryo lethality was reported for mice administered 2-mercaptobenzothiazole at a dosage of 200 mg/kg in corn oil by intraperitoneal injection on days 1 through 15 of gestation.

2-mercaptobenzothiazole was evaluated in the L5178Y TK mouse lymphoma mutation assay and in microbial mutagenicity assays. The microbial assays employed five strains of Salmonella and one yeast strain. No mutagenic effects were demonstrated in these assays, either with or without mammalian microsomal activation.

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TH EFFECTS SUMMARY (continued)

ditional Ames/Salmonella assays on 2-mercaptobenzothiazole have been reported
veral manufacturers and by the National Toxicology Program. With the
tion of one equivocal positive finding in one Salmonella strain in one
, the results on 2-mercaptobenzothiazole have been uniformly negative in
nella mutagenicity assays.

vidence of genotoxic activity was found in either the CHO/HGPRT cell point
ion or BALB/C 3T3 cell transformation assays. A micronucleus assay was
rmed in CD-1 mice at a dose level of 300 mg/kg; no evidence of clastogenic
ity was seen in this assay. A weak positive result, occurring only at
y cytotoxic doses, was reported for 2-mercaptobenzothiazole in the L5178Y TK
lymphoma assay.

ercutaneous absorption of ¹⁴C-labelled 2-mercaptobenzothiazole (11 mg/kg)
ving application to intact and abraded skin of guinea pigs was determined by
ement of radioactivity in urine, feces, blood, gastrointestinal tract and
al organs. After 48 hours, recovery from these fluids and tissues was
rimately 9% and 37% of the administered dose for intact and abraded animals,
ctively. Following administration of ¹⁴C-labelled 2-mercaptobenzothiazole
cutaneous injection, 90% of the administered dose was recovered in the
as glucuronide or sulfate conjugates and 9% appeared as unchanged 2-mercap-
thiazole during a 6 hour post-injection period.

ditional Toxicology Program (NTP) reported the results of a carcinogenicity
ay with 2-mercaptobenzothiazole (MBT) in Fischer 344/N rats and B6C3F1
Fifty animals of each species and sex were administered MBT in corn oil by
5 days per week for 103 weeks. Rats were given 0, 375 and 750 mg/kg/day
ce were given 0, 188 and 375 mg/kg/day. The NTP report concluded that
was some evidence of carcinogenic activity" in male and female rats. Male
howed an increased incidence of mononuclear cell leukemias and pancreatic
adenomas at the low dose only; adrenal gland pheochromocytomas were more
nt in treated than control animals. Female rats showed an increased
nce of pituitary adenomas on both treatment groups. There was no evidence
cinogenicity in male mice. The NTP report concluded that there was "equi-
vidence for carcinogenic activity" on the basis of an increased incidence
atocellular adenomas in female mice in the low dose group only. The tumor
reported are commonly observed as spontaneous lesions in these species and
s, and the significance of the increased incidence seen in treated animals
ertain due to the possible adverse effects of the use of excessive dose
ns and corn oil vehicle gavage.

or mercaptobenzothiazole disulfide

D₅₀ (Rat): >7,940 mg/kg, Practically Nontoxic
LD₅₀ (Rabbit): >7,940 mg/kg, Practically Nontoxic
ritation (Rabbit): (FHSA) 0.6 on a scale of 110.0, Practically Nonirritating
rritation (Rabbit): (FHSA) 0.0 on a scale of 8.0, Nonirritating

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HEALTH EFFECTS SUMMARY (continued)

Patch testing of 53 human volunteers with mercaptobenzothiazole disulfide as a 70% preparation in petrolatum, produced no positive reactions following the initial application, any of the 15 serial applications, or in challenge applications 2 weeks later. Mercaptobenzothiazole disulfide was not considered a primary or cumulative irritant or a sensitizing agent.

Mercaptobenzothiazole disulfide (MBTS) was evaluated for toxicity in studies in which 2 groups of mice were given either a single subcutaneous injection of the test material at a dosage of 1,000 mg/kg followed by observation for 78 weeks, or 464 mg/kg of the test material by oral intubation for 21 days followed by administration of a diet containing MBTS at concentrations equivalent to 205 mg/kg/day for 77 weeks. No adverse effects were reported, and no statistically significant increases in tumor incidences were observed in either study.

The teratologic potential of mercaptobenzothiazole disulfide (purity unspecified) was evaluated in a study in which rats and mice were dosed at 10 or 100 mg/kg/day (by oral gavage) on gestation days 8 - 12, 13 - 17 or 1 - 21. Teratologic effects were reported in mice and rats of the high-dose group. Rats were reported to have significant increases in post-implantation mortality and decreased fetal weight when MBTS was administered at 100 mg/kg on gestation days 13 - 17 or 1 - 21; malformations, including intracranial hematomas and hydrocephalus, were noted. No fetotoxic or embryotoxic effects were seen in mice, but hydrocephalic malformations were reported as elevated. Maternal toxicity was observed in those animals receiving 100 mg MBTS per kg of body weight per day. No embryotoxic or teratologic effects were observed at 10 mg/kg in either rats or mice.

Mercaptobenzothiazole disulfide of unknown purity was administered by gavage to rats at 200 mg/kg on days 4 and 11 of gestation. Following sacrifice on day 19 of gestation, examinations for embryonic mortality were performed. Total embryonic mortality and post-implantation losses were reportedly increased after treatment.

An increase in total embryonic and post-implantation mortality was reported in a dominant lethal study conducted with mercaptobenzothiazole disulfide using female rats administered dosages of 2,000 mg/kg on day 1 and 3 of estrus and males administered the same dose twice in a 3 day period prior to mating.

Mercaptobenzothiazole disulfide was evaluated in the L5178Y TK mouse lymphoma mutation assay and in microbial mutagenicity assays. The microbial assays used five strains of Salmonella and one strain of yeast. No mutagenic effects were demonstrated.

Mercaptobenzothiazole disulfide was also evaluated for mutagenic or genotoxic potential in the following systems: microbial assays with S. typhimurium strains, BALB/C 3T3 cell transformation assay, and *in vitro* Chinese hamster ovary (CHO) cell point mutation and chromosome aberration assays. MBTS was reported to be positive in the BALB/C 3T3 cell transformation assay. No evidence of mutagenicity was observed in any of the other assays.

PHYSICAL DATA

Appearance: Light tan to buff powder or pellets
Odor: Slight amine
Melting Point: Approximately 102°C
Specific Gravity @ 25°C/4°C: Approximately 1.3
Solubility in Water: Insoluble
 in Acetone: Soluble
 in Hexane: Approximately 1.7 g/100 ml
 in Alcohol: Approximately 5.6 g/100 ml @ 28°C

NOTE: These physical data are typical values based on material tested but may vary from sample to sample. Typical values should not be construed as a guaranteed analysis of any specific lot or as specifications for the product.

SPILL, LEAK & DISPOSAL INFORMATION

Waste Disposal: When discarded, SANTOCURE vulcanization accelerator is not a "hazardous waste" as that term is defined in 40 CFR 261, "Identification and Listing of Hazardous Waste." Burn in an approved incinerator or dispose of in an approved chemical landfill in accordance with all applicable local, state and federal laws and regulations. Consult your attorney or appropriate regulatory officials for information on such disposal.

Spill or Leakage Procedures: Vacuum or sweep up and place in dry, covered container for disposal as recommended above. Flush area with water.

Containers: Burn in an approved incinerator or dispose of in an approved chemical landfill in accordance with all applicable local, state and federal laws and regulations.

ADDITIONAL COMMENTS

SANTOCURE vulcanization accelerator slowly degrades on storage particularly under warm, humid conditions. Keep stocks below 40°C, dry and away from sunlight. Keep containers closed. Use stocks within 6 months of receipt.

For further information on sulfenamide storage and handling, consult the Monsanto Rubber Chemicals Division publication, "Rubber Chemicals Stability."

Environmental Toxicity Information:

96-hr LC₅₀ Rainbow Trout: 5.4 mg/l, Moderately Toxic
96-hr LC₅₀ Bluegill: 7.9 mg/l, Moderately Toxic
96-hr LC₅₀ Fathead Minnow: >1,000 mg/l, Nontoxic
48-hr LC₅₀ Daphnia: 18 mg/l, Slightly Toxic
96-hr EC₅₀ Algae, Cell Count: 1.1 mg/l, Moderately Toxic

For additional information consult the Monsanto Rubber Chemicals Purchasing Guide.

Monsanto MATERIAL SAFETY DATA
SANTOCURE® VULCANIZATION ACCELERATOR

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DATE 6/87

SUPERSEDES 4/86

MSDS NUMBER 000065330

FOR ADDITIONAL NON-EMERGENCY INFORMATION, CONTACT:

Manager, Product Safety
Monsanto Chemical Company
Rubber Chemicals Division
314-694-1000

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Place Syracuse New York
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