1-6-93

DATE OUT: _____

DP BARCODE: D185106 **SUBMISSION:** S430115 **REREG CASE #:** 3148
CHEMICAL CODE/NAME: 107401 3-(Trimethoxysilyl)propyl dimethyl octadecyl ammonium chloride (Trimethoxylsilyl quats) **CAS #:** 27668-52-6

REGISTRATION DIVISION/REGISTRATION SUPPORT BRANCH/PRODUCT CHEMISTRY REVIEW SECTION TRANSMITTAL/PRODUCT CHEMISTRY REVIEW OF A REREGISTRATION ACTION FOR A TECHNICAL GRADE ACTIVE INGREDIENT PHASE IV [X], V [ ], OR MISCELLANEOUS DATA [ ]

Data Submitter: 034292 Dow Corning Corp. **Subm. Date:** 09/25/92

SRRD PM#/NAME: 53 Bruce Sidwell **Phone #:** 308-8078
SRRD CRM NAME: Margarita Collantes **Phone #:** 308-8583

CONCLUSIONS/ISSUES REMAINING TO BE RESOLVED:

1. The registrant will need to submit product chemistry data requirements cited in this report as GLR # 63-4 (Odor).

2. The registrant will need to upgrade product chemistry data requirements of GLR #'s:

   (a) 63-5 (Melting Point) using the technical grade active ingredient, a solid material in methanol; and

   (b) 63-8 (Solubilities) by reporting the amount of AI soluble in grams per 100 ml of a solvent.

3. The submitted storage stability for Dow Corning 5700 Antimicrobial Agent, a requirement of GLR #63-17 is adequate. No additional data is needed for this topic.

4. In all the required testings to satisfy generic data requirements using a manufacturing-use product, the AI must be isolated. If it is not possible, the practical equivalent of the TGAI must be reported. For example, if the solubility of a 42% AI is 8.4 gm/100 ml, the practical equivalent would be 20 gm/100 ml.

5. The registrant will need to submit an updated label expressing the active ingredient in nominal in accordance with PR Notice 91-2; and a CSF for the TGAI listing the upper and lower limits of the technical grade active ingredient and the upper limits for all others.

6. N,N-dimethylnitrosamine was not detected in Dow Corning Q9-5700 Antimicrobial Agent (< method detection limit of 230 ppb).

7. We defer to TOX/HED for their concern with the following three impurities in technical 107401 3-(Trimethoxysilyl)propyl dimethyloctadecyl ammonium chloride: (a) Octadecyldimethylamine (2%), (b) chloropropyltrimethoxysilane (16.6%), and (c) 3-(trimethoxysilyl)propane (0.2%).

NOTES TO PM:

(1) A Status Report of Product Chemistry Data Requirements is Included on page 2; and
(2) Information in Appendix A is confidential (pages 8 to 12 pages), and
(3) Please note our deferral to TOX/HED (Conclusion 7).

Sami Malak
Reviewer: Sami Malak, Chemist — **12/30/92** **Date**

D. Stubbs
Section Head: Don Stubbs, Acting — 1/6/93 **Date**

1

STATUS REPORT OF PRODUCT CHEMISTRY DATA REQUIREMENTS FOR REREGISTRATION OF A TECHNICAL GRADE ACTIVE INGREDIENT

DP BARCODE #: D185106 SUBMISSION #: S430115 REREG CASE #: 3148 DATE: 12/30/92
CHEMICAL NAME: 107401 3-(Trimethoxysilyl)propyl dimethyl octadecyl ammonium chloride
COMMON NAME: Trimethoxysilyl quats CAS #: 27668-52-6

GLR #	TITLES	Ac	NA	UP	Dg	MRID No.
	Series 61-Product Identity and Composition (40CFR§158.155, 160, 162, 165 & 167)					
61-1	Product Identity & Disclosure of Ingredients	X				932180-01C, 424565-01, 424565-02, 932180-22 & 932180-30
61-2	Description of Starting Materials & Manufacturing Process	X				
61-3	Discussion of Formation of Impurities	X				
	Series 62-Analysis and Certification of Product Ingredients (40CFR§158.170, 175 & 180)					
62-1	Preliminary Analysis of Product Samples	X				424565-03 424565-04, 424565-05, 424565-06, 424565-06 & 425565-07
62-2	Certification of Ingredient Limits	X				
62-3	Analytical Methods to Verify Certified Limits	X				
	Series 63-Physical and Chemical Characteristics (40CFR§158.190)					
63-2	Color	X				~~424969-01~~ ? 424565-08, 424565-09, 424565-10, 932180-04C & 932180-04
63-3	Physical State	X				
63-4	Odor				X	
63-5	Melting Point			X		
63-6	Boiling Point	X				
63-7	Density, Bulk Density, or Specific Gravity	X				
63-8	Solubility			X		
63-9	Vapor Pressure		X			
63-10	Dissociation Constant		X			
63-11	Octanol/Water Partition Coefficient		X			
63-12	pH	X				
63-13	Stability	X				
64-1	Submittal of Samples		X			

61-1 Confirmed

EXPLANATIONS:: AC = Acceptable; NA = Not Applicable/Waiver Acceptable; Up = Needs upgrading; Dg = Data Gap; GLR# = Guideline Reference Number; TGAI = Technical Grade Active Ingredient; PAI = Pure Active Ingredient; MP = Manufacturing-Use Product; EP = End-Use Product; CBI = Confidential Business Information.

NOTES: 62-1 Required of all technicals undergoing reregistration.
62-3 EPA validated method may be referenced from published sources.
63-5 Required if the TGAI is a solid at room temperature.
63-6 Required if the TGAI is a liquid at room temperature.
63-11 Required if the TGAI is organic and non-polar.
63-12 Required if test substance is dispersible with water.
64-1 Samples of a TGAI and PAI are required on a case-by-case basis

DP BARCODE:D185106 **SUBMISSION:**S430115 **REREG CASE #:** 3148
CHEMICAL CODE/NAME:107401 3-(Trimethoxysilyl)propyl dimethyl octadecyl ammonium chloride (Trimethoxylsilyl quats) **CAS #:**27668-52-6

Detailed Considerations

NOTES:

1. Several statements of data confidentiality were included with this submission claiming confidentiality of some of the data on the basis of its falling within the scope of FIFRA§10(d)(1)(A), (B), or (C). Data requirements of GLR #'s 61-2, 61-3, 62-1, and 62-2 are CBI which, is reviewed in Confidential Appendix A.

2. Several GLP statements were included with this submission to the effect that some studies meet meet the requirements of FIFRA §610, while other do not. Some data were generated prior to the advent of GLP Guidelines.

3. Included with this submission were:

   (a) A LUIS report, dated 9/25/91, for chemical 107401 3-(Trimethoxysilyl)propyl dimethyl octadecyl ammonium chloride, CAS #27668-52-6.

   (b) Phase 3 registrant's response work sheets, dated 07/17/90, indicating that data is provided or correspondences are attached.

   (c) Phase 2 review by B. Gandhi, dated 5/2/90.

   (d) Phase 2 draft addendum report, dated 06/20/90. The report reflects Gandhi's memo (#3 above) in which the registrant's request for a data waiver of some requirements were denied unless supported by scientific or regulatory reasons.

PRODUCT CHEMISTRY DATA REQUIREMENTS

Series 61 Product Identity and Composition

MRID #'s 424565-08: Data submitted in MRID #424565-08C is entitled "Phase 3 Submission of revised MRID 00070190 Product Bulletin: Information About Antimicrobial Agents: Dow Corning Q9-5700 Antimicrobial Agent." The study was authored by E. A. Abbott of Dow Corning Corporation, dated 7/17/90, 15 pages.

Data submitted in MRID #932180-01C is entitled "Phase 3 Summary of MRID #'s 00130316 and Related MRID's 00164909 and 00070190 and Dow Corning 5700 Antimicrobial Agent and Dow Corning 5772 Antimicrobial

Agent Registration Correspondence". The study was prepared by W. C. White; original study was prepared by Dow Corning Corporation, dated 12/21/90, 8 pages.

61-1 Product Identity & Disclosure of Ingredients

Chemical Name: 107401 3-(Trimethoxysilyl)propyl dimethyl octadecyl ammonium chloride

Common Name: Trimethoxylsilyl quats

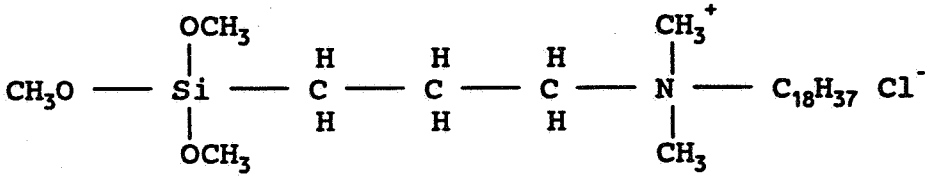
CAS No. 27668-52-6

Molecular Weight: 497.5

Molecular Formula: $[CH_3O)_3Si(CH_2)_3N(CH_3)_2C_{18}H_{37}]^+Cl^-$

Empirical Formula: $SiC_{26}H_{58}O_3NCl$

Structural Formula:



61-2 Description of Beginning Materials & Manufacturing Process
See Confidential Appendix A.

61-3 Discussion of Formation of Impurities
See Confidential Appendix A.

Series 62 Analysis and Certification of Product Ingredients

MRID #424565-07: Data submitted is entitled "Phase 3 New Submission of Supplemental Materials: Batch Analysis Report For Dow Corning 5700 Antimicrobial Agent and Dow Corning 5772 Antimicrobial Agent." The studies were authored by J. R. Malek and R. J. Robinson; original studies were presented by Dow Corning Corporation, dated 9/13/78, Volume IX, 10 pages.

62-1 Preliminary Analysis of Product Samples
See Confidential Appendix A.

62-2 Certification of Ingredient Limits
See Confidential Appendix A.

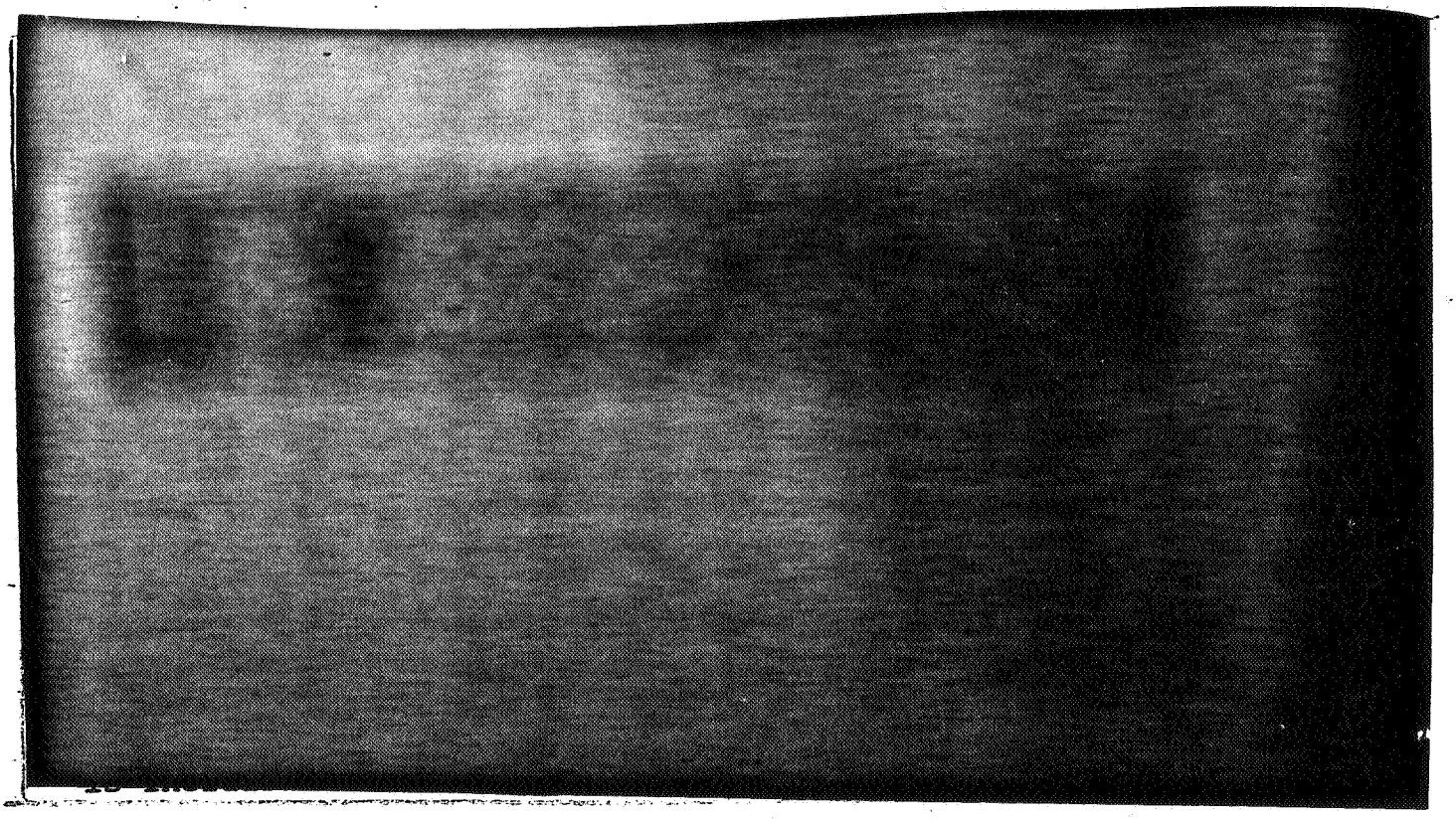
62-3 Analytical Method to Verify Certified Limits

NOTE: Methods for impurities are CBI, please refer to Appendix A.

Method for the Technical Grade Active Ingredient

Corporate Test Method (CTM) 0230, MRID #424565-03

The method entitled "Phase 3 Submission of Supplemental Materials: Corporate Test Methods 0230." The method is authored by James R. Malek; original study was presented by Dow Corning Corporation, dated 7/13/90, Vol. IV, 14 pages.



Series 63 Physical and Chemical Characteristics

MRID #'s 424969-01 & 932180-04C Data submitted in MRID #932180-04C is entitled "Phase 3 Summary of MRID 00070190 and Related MRID's #00130316 and Supplemental Data 129565, Physical and Chemical Characteristics." The studies were summarized by W. C. White; original study prepared by Dow Corning Corporation of Midland, Michigan, dated 07/16/90, 11 pages.

Data submitted in MRID #424969-01 is entitled "Phase 3 Revision of Summary of MRID 00070190 and Related MRID's #00130316 and Supplemental Data 129565, Physical and Chemical Characteristics." The studies were summarized by W. C. White; original study prepared by Dow Corning Corporation of Midland, Michigan, dated 07/13/90, 70 pages.

QUALITY CONTROL PROCEDURE INFORMATION IS NOT INCLUDED

63-2 Color: Light to dark amber.

63-3 Physical State: liquid at 20°C.

63-4 Odor: No data was submitted.

63-5 Melting Point: Not applicable. The TGAI is liquid.

63-6 Boiling point: 64°C.

63-7 Density, Bulk Density, or Specific Gravity: 0.841 to 0.859

63-8 Solubility: At room temperature, the product is miscible in all proportions with water, alcohols, ketones, esters, hydrocarbons, and chlorinated hydrocarbons.

63-9 Vapor Pressure: Not applicable. The TGAI is a reactive silane which polymerizes in the presence of moisture.

63-10 Dissociation Constant: Not applicable. The TGAI is a cationic with hydrolyzable alkoxy silane functionality. As a cationic quaternary ammonium salt, the TGAI will completely ionize in an aqueous solution.

63-11 Octanol/Water Partition Coefficient: Not applicable. The TGAI is highly polar.

63-12 pH: 5.3 to 6.9 at 20°C.

63-13 Stability: (MRID #'s424969-01, 424969-01, 932180-04C, 424565-09) - Only thermostability was conducted showing stability of the TGAI to elevated temperatures with slow decomposition reported at 125°C. Further, exposure to ambient light showed no changes in the test substance. No stability tests were conducted, however, for metals, metal ions since, according to the registrant, packaging and use of the product does not encounter metals or metal ions.

PRODUCT LABEL:

One label was included with this submission for Dow Corning Q9-5700 Antimicrobial Agent, Reg. No. 34292-1, accepted on 7/16/76. The active ingredient was reported at 42% in methanol. The percentage by weight on products labels should be expressed in nominal in accordance with PR Notice 91-2.

Product Specific Data

Storage Stability: MRID #424565-10

A storage stability study that should have been submitted in response to the Product Specific DCI's is reviewed here as part of the requirements for reregistration.

The submitted study is entitled "Phase 3 Submission Supplemental Data: Storage Stability Data For Dow Corning Antimicrobial Agent." The study was authored by S. Gardner; original study was prepared by Dow Corning Corporation, Vol. XIII, dated 12/10/84, 12 pages.

In the submitted study five samples from two lots of Dow Corning 5700 Antimicrobial Agent were stored under room temperature for a period of 14 months. Analysis for total amines and the quat salt showed no changes in the contents at the conclusion of the study.

Attachments: Confidential Appendix A (pages 8 to 12).

cc With Attachment: S. Malak and Central File (Rereg Case No.3148).
H7505C:RD:RSB:PCRS:CM#2:S. Malak:Rm711I:s.m.:12/30/92:305-6361:C3148A

TRIMETHOXYSILYL QUATS PC 107401

Page_____ is not included in this copy.

Pages 8 through 12 are not included.

The material not included contains the following type of information:

____ Identity of product inert ingredients.

____ Identity of product impurities.

✓ Description of the product manufacturing process.

✓ Description of quality control procedures.

____ Identity of the source of product ingredients.

____ Sales or other commercial/financial information.

____ A draft product label.

____ The product confidential statement of formula.

____ Information about a pending registration action.

____ FIFRA registration data.

____ The document is a duplicate of page(s) _____.

____ The document is not responsive to the request.

The information not included is generally considered confidential by product registrants. If you have any questions, please contact the individual who prepared the response to your request.