AR226 – 3269

Determination of Ultraviolet Spectrum: [redacted]

DUPONT REPORT # 12734

[redacted] **ULTRAVIOLET SPECTRUM**

Test Guideline(s)

Authors

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Study Completion Date

16 July 2002

Report Date

21 March 2003

Test Facility

DuPont Corporate Center for Analytical Sciences

Experimental Station 402/5321 and E328/162B

Wilmington, DE 19880

Sponsor

Telomer Research Panel
c/o Rand Corporation

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1.0 Summary

Test System:

[redacted] was used to determine its ultraviolet spectrum at 25°C.

Findings:

There is no measurable absorption from 225 to 400 nm.

Conclusions:

There is no measurable UV absorption for this compound.

2.0 General Study Information

Study Objectives

The objective of this study was to determine the ultraviolet absorption spectrum of [redacted] at 25°C.

Test System Justification

The test system was selected by the sponsor.

Study Personnel

Management:	Marianne Marsi, Ph.D.
Study Director:	Mary A. Kaiser, Ph.D.
Principle Investigator:	Raymond E. Richardson
Technical Personnel:	Raymond E. Richardson

Study Execution Dates

Study Initiation Date:	15-Jun-2001
Experimental Start Date:	15-Jun-2001
Experimental Completion Date:	28-June 2002
Study Completion Date:	12-July 2002

3.0 MATERIALS AND METHODS

3.1 Test Guidelines

OECD Guidline 101 ws used in this study. The ultraviolet absorption spectrum of a solution is a function of the concentration, c_i, expressed in mol/L, of all absorbing species present; the path length, d, of the spectrophotometer cell, expresed in cm; and the molar absorptivity (extinction coefficient), ϵ_i, of each species. The absorbance (optical density) A of the solution is then given by

$$A = d \sum_i \epsilon_i, c_I$$

3.2.1 Chemical System

3.2.1.1 Test Substance

The test substance was obtained from Clariant Gmbh (Germany) and was shown to be [redacted] pure via gas chromatography. [redacted] impurities were detected. The major impurity [redacted] was tentatively identified as [redacted] based on the mass spectral fragmentation pattern

Name:

Synonym:

Active substance(s)

CAS Name:

[redacted]

CAS Number(s):

Structure:

[redacted]

Company Sanitized. Does not contain TSCA CBI

Determination of Ultraviolet Spectrum: 8-2 Telomer B Alcohol

H Number	H-24691
Lot Number:	[redacted]
EMSE Sample Number:	E93386-63
Concentration, nominal:	[redacted]
Concentration, analyzed:	
Certificate of Analysis Date:	03-Apr. 2001
Date Received:	15-June -2001
Solubility at 25°C.:	~140 $\mu g\ L^{-1}$
Vapor pressure:	0.023 mm Hg
Stability:	Stable at ambient room temperature
Appearance/Color:	White solid
Storage Conditions:	Room temperature; keep tightly closed

3.2.1.2 Test Vehicle

The test substance was [redacted] dissolved in spectrophotometic-grade methanol.

3.3 Test Conduct

The [redacted] was dissolved in methanol. A Varian Cary 5 ultraviolet/visible/near-infrared spectrophotometer was used to obtain the spectrum. The sample was weighed into a 10-mL class A volumetric flask and brought to volume with spectrophotometric-grade methanol. The solution was shaken and examined visually to ensure that there were no insoluble materials. Two 1-cm cells were triple rinsed with methanol then filled with methanol and placed in the sample and reference beams of the Cary 5 spectrophotometer. A baseline was collected in methanol versus methanol to ensure compensation. The sample cell was then emptied and rinsed three times with sample solution before filling with fresh sample. The sample cell was then placed in the sample beam and the spectrum recorded versus methanol.

3.4 Parameters Observed

Changes in molar absorbtivity ($M^{-1}\ cm^{-1}$) were recorded versus wavelength (nm).

3.5 Result Analysis

The output was compared to the spectrum of methanol versus methanol. Any observable absorption above baseline is noted in the report.

3.6 Validity Criteria of the Study

The instrument was calibrated for both wavelength accuracy and photometric accuracy

3.7 *Protocol Deviations*

None

4.0 RESULTS AND DISCUSSION

The ultraviolet absorption spectrum showed no absorption within the wavelength region measured.

5.0 CONCLUSIONS

[redacted] does not absorb ultraviolet radiation in this range.

6.0 RETENTION OF RECORDS

Study documents and materials will be stored in the archives of the DuPont Experimental Station including but not limited to:

- study protocol;
- any protocol and/or report amendments or addenda or deviations;
- all raw data;
- one original signed copy of the final report;
- laboratory-specific or site-specific raw data such as personnel files, instrument, equipment, refrigerator, and/or freezer raw data.

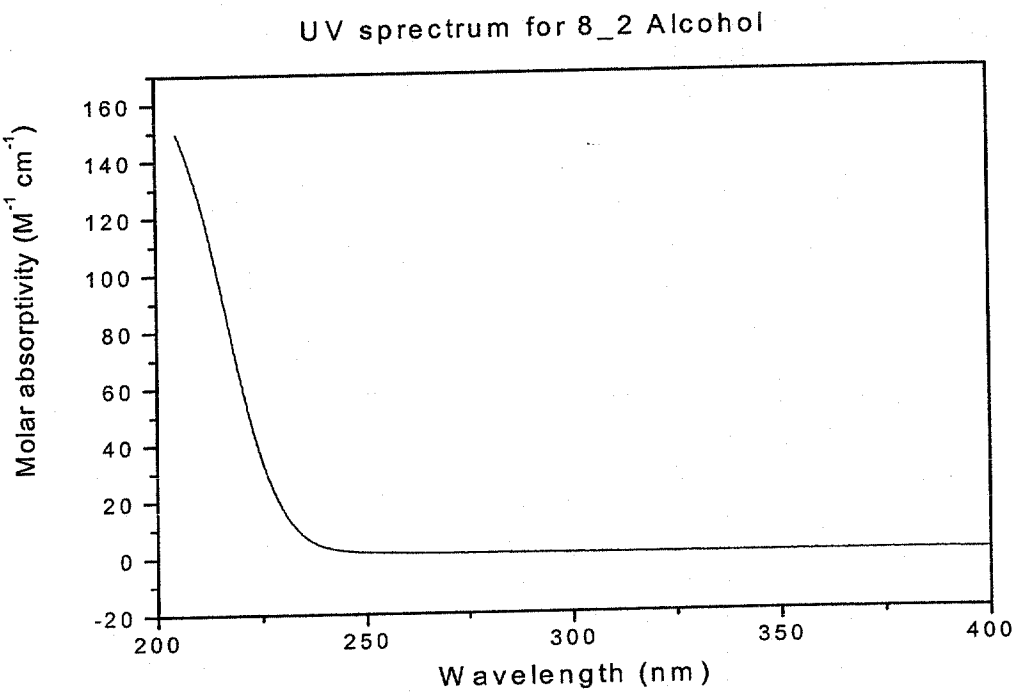
7.0 DISPOSAL OF TEST ITEM

After issuance of the final report, the remaining test substance will be stored at the DuPont Glasgow site until its expiration date and then destroyed by burning, unless other arrangements are made between the sponsor and the Test Facility.

8.0 REFERENCE

OECD Guideline for Testing of Chemicals 101, adopted 12 May 1981,UV-VIS Absorption Spectra (Spectrophotometric method).

Figure 1. Ultraviolet Absorption Spectrum of [redacted] at 25°C.



Determination of Ultraviolet Spectrum: [redacted]

Appendix A

Chemical Analysis Summary

[redacted]

H-24691

Analysis Summary

The subject material was analyzed by gas-chromatography using a standard method to assess its composition. This analysis showed that the material comprised [redacted] of the subject material. The balance [redacted] was not [redacted] at a limit of quantitation of 0.02%. Further analysis by GC/MS suggested that the [redacted] was a single impurity, whose chemical structure is [redacted]

Finally, the subject material was evaluated by High Performance Liquid Chromatograpy - Tandem Mass Spectrometry (LC/MS/MS) for the presence of perfluorooctyl sulfonic acid and perfluorooctanoic acid at a detection limit of 0.1ppm. Neither material was observed to be present.

Material	Wt. % (±0.3)
[redacted]	

Company Sanitized. Does not contain TSCA CBI