Reconsile Consortium:
Substance Identification Profile for N-(3-(trimethoxysilyl)propyl)ethylenediamine

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Date: 7th March 2012
Record of report finalisation

Conclusions drawn and recommendations made in this report represent the unbiased view of Peter Fisk Associates on the basis of the data presented and obtained.

The signature below confirms that this version of the report is complete and final.

Signed on behalf of Peter Fisk Associates

…………………………………………………….

Dr. Peter Fisk

Date …………………………………………………
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Reconsile Consortium:  
Substance Identification Profile for  
N-(3-(trimethoxysilyl)propyl)ethylenediamine

Substance Identification Profile

The substance identification profile for N-(3-(trimethoxysilyl)propyl)ethylenediamine (CAS 1760-24-3, EC 217-164-6) applicable to the Reconsile Consortium at the date of this report is:

- Molecular weight: 222.36 g mol\(^{-1}\)
- Structure and SMILES code

\[
\text{NCCNCC[Si](OC)(OC)OC}
\]

- Purity: \(\geq 80\%\)
- Deviations below this purity value may be acceptable but should they occur a company should assess their statistical significance and submit new information if necessary.
- Hydrocarbon and alkoxy silane impurities have been identified.
- No definite SVHC constituents are present.

The basis of the profile is described in the sections following this summary.
1. **Introduction and methods**

The substance N-(3-(trimethoxysilyl)propyl)ethylenediamine (CAS 001760-24-3, EC 217-164-6) may be registered by one or more members of the REACH Consortium known as Reconsile. This report concerns review of compositional data provided to Peter Fisk Associates for review, in order to establish the sameness (comparability) of samples from different suppliers (manufacturers or importers).

It consists of a brief review of the information provided by each legal entity, in confidential annexes, and a generic non-confidential substance identification profile (SIP). Reconsile members having identified certain information entered in IUCLID 5 as confidential, such as impurity profiles, should inform PFA accordingly so that the confidentiality can be maintained in the SIP.

This SIP assists with demonstration of
- Valid sharing of studies from different companies, as far as reasonably practicable
- pre-SIEF consortium arrangements and for the SIEF itself, inclusion of any non-Reconsile ‘joiners’.

It may be of use in the Reach Registration process for individual registrants, but that is not its primary purpose.

Should it be the case that during review, the authors of this report wished to exclude a substance from one or more suppliers on grounds of lack of sameness (despite use of the same EINECS number by the suppliers), then the authors will have discussed that with the suppliers, but no report of that has been included in this report.

This report does not include the reports or spectra provided by the individual companies, but does reference the sources.

1.1 **Analytical characterisation to confirm substance identity.**

(From the ECHA Guidance for identification and naming of substances under REACH).

When a registration is required under REACH it shall include information on the identification of the substance as specified in item 2 of Annex VI (see table 1). This information shall be adequate to enable each substance to be identified sufficiently.

A “mono-constituent” substance (one constituent >80%) is completely identified by its chemical composition, the chemical identity and the content of each constituent in the substance (identification parameters).

If it is not technically possible, or if it does not appear scientifically necessary, to give information on one or more of the substance identification parameters, the reasons shall be clearly stated in the form of an expert statement.

The analytical characterisation should on this basis confirm the identity of the substance, by defining its chemical composition.
Table 1: Substance identification parameters in REACH Annex VI item 2:

<table>
<thead>
<tr>
<th></th>
<th>IDENTIFICATION OF THE SUBSTANCE</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>For each substance the information given shall be sufficient to enable each substance to be identified. If it is not technically possible or if it does not appear scientifically necessary to give information on one or more items below, the reason shall be clearly stated.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>2.1</th>
<th>Name or other identifier of each substance</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1.1</td>
<td>Name(s) in the IUPAC nomenclature or other international chemical name(s)</td>
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<tr>
<td>2.1.2</td>
<td>Other names (usual name, trade name, abbreviation)</td>
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<tr>
<td>2.1.3</td>
<td>EINECS or ELINCS number (if available and appropriate)</td>
</tr>
<tr>
<td>2.1.4</td>
<td>CAS name and CAS number (if available)</td>
</tr>
<tr>
<td>2.1.5</td>
<td>Other identity code (if available)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>2.2</th>
<th>Information related to molecular and structural formula of each substance</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.2.1</td>
<td>Molecular and structural formula (including SMILES notation, if available)</td>
</tr>
<tr>
<td>2.2.2</td>
<td>Information on optical activity and typical ratio of (stereo) isomer (if applicable and appropriate)</td>
</tr>
<tr>
<td>2.2.3</td>
<td>Molecular weight or molecular weight range</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>2.3</th>
<th>Composition of each substance</th>
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<td>2.3.1</td>
<td>Degree of purity (%)</td>
</tr>
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<td>2.3.2</td>
<td>Nature of impurities, including isomers and by-products</td>
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<tr>
<td>2.3.3</td>
<td>Percentage of (significant) main impurities</td>
</tr>
<tr>
<td>2.3.4</td>
<td>Nature and order of magnitude (.....ppm, ......%) of any additives (e.g. stabilising agents or inhibitors)</td>
</tr>
<tr>
<td>2.3.5</td>
<td>Spectral data (ultra-violet, infra-red, nuclear magnetic resonance or mass spectrum)</td>
</tr>
<tr>
<td>2.3.6</td>
<td>High performance liquid chromatogram, gas chromatogram</td>
</tr>
<tr>
<td>2.3.7</td>
<td>Description of the analytical methods or the appropriate bibliographical references for the identification of the substance and, where appropriate, for the identification of impurities and additives. This information shall be sufficient to allow the methods to be reproduced.</td>
</tr>
</tbody>
</table>

1.2 Reconcile substances: appropriate analytical information

- **Sufficient spectral data** are needed to confirm the structure given for a mono-constituent substance or to confirm that a reaction mixture is not a preparation.
- **Spectroscopic methods** see below
- **Chromatographic methods**, such as Gas Chromatography (GC) or High-Performance Liquid Chromatography (HPLC) are needed to confirm the composition of the substance. An appropriate chromatogram will confirm the existence of impurities, additives and the constituents of a reaction mixture.
- If appropriate, also other valid constituent separation techniques may be used. Spectroscopic and analytical methods are subject to continuous change. Therefore, it is the responsibility of the registrant to present appropriate spectral and analytical data.
- REACH requires the registrant to describe the analytical methods and/or to provide the bibliographical references for the methods used for identification of the substance and, where appropriate, for the identification of impurities and additives. This information should be sufficient to allow the methods to be reproduced.
The agreed application of these principles within the Reconsile Consortium:

- NMR (at least one of $^{29}\text{Si}$, $^{13}\text{C}$, $^1\text{H}$) would usually be useful
- GC-MS or GC and MS: essential.
- IR would usually be useful

UV-Vis would most of the time not be needed for Si based materials due to the absence of chromophores (an expert statement may be required).

In addition
1. GLP is not required for the analytical characterisation;
2. Impurities should be identified if $>or=1\%$;
3. SVHC impurities should be identified if $>or=0.1\%$ if there are grounds to believe based on expert review that they might be present, for example due to the manufacturing process.

As general methodology, the lowest purity from a company causes a purity to be set in the SIP according to the following:

<table>
<thead>
<tr>
<th>Lowest</th>
<th>Rounded down to</th>
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<tbody>
<tr>
<td>80-85</td>
<td>80</td>
</tr>
<tr>
<td>85.1-90</td>
<td>85</td>
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<tr>
<td>90.1-93</td>
<td>90</td>
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<tr>
<td>93.1-95</td>
<td>93</td>
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<td>95.1-97</td>
<td>95</td>
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<td>97.1-98</td>
<td>97</td>
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<tr>
<td>98.1-99</td>
<td>98</td>
</tr>
<tr>
<td>99.1-99.5</td>
<td>99</td>
</tr>
<tr>
<td>99.6-100</td>
<td>99.5</td>
</tr>
</tbody>
</table>

This gives some flexibility. In addition, it should be noted that suppliers were asked to analyse samples of their highest grade commercial products. When a company sells a product of lower purity than the SIP, then they have to ensure that they take any steps to ensure valid use of the shared data.
2. Information available for N-(3-(trimethoxysilyl)propyl)ethylenediamine

This section gives the basis of the substance identification profile.

2.0 Companies with an interest in the SIP

Dow Corning Europe SA
Evonik Degussa GmbH
Momentive Performance materials GmbH
Shin Etsu Silicones Europe BV
Wacker Chemie AG

The exact legal entities with responsibility for the substance, as defined by the REACH Regulation, are the responsibility of these companies themselves. The SIP is based on the information available from the companies, described in section 2.3. All of the companies with an interest in the substance have provided data.

2.1 Substance Identifiers

2.1.1 Name

N-(3-(trimethoxysilyl)propyl)ethylenediamine

2.1.2 Other Names

The relevant parts of the CAS Registry File entry (on 11th February 2011) for the substance follow unamended:

Display from REGISTRY

ANSWER 1 © 2011 ACS on STN

Structure Diagram

Chemical Name
1,2-Ethanediamine, N1-[3-(trimethoxysilyl)propyl]- (CA INDEX NAME)
1,2-Ethanediamine, N-[3-(trimethoxysilyl)propyl]- (9CI)
Ethylenediamine, N-[3-(trimethoxysilyl)propyl]- (6CI, 7CI, 8CI)
(.beta.-Aminoethyl).gamma.-aminopropyltrimethoxysilane
(.gamma.-Ethylenediaminepropyl)trimethoxysilane
(2-Aminoethyl)(3-(trimethoxysilyl)propyl)amine
(Trimethoxysilylpropyl)ethylenediamine
.gamma.-2-Aminoethylaminopropyltrimethoxysilane
.gamma.-Ethylenediamino)propyltrimethoxysilane
3-(N-Aminoethyl)aminopropyltrimethoxysilane
3-(Trimethoxysilyl)propylethylenediamine
3-[N-(2-Aminoethyl)amino]propyltrimethoxysilane
6-Amino-4-azahexyltrimethoxysilane
A 0700
A 1120
A 1122
A 1200
A 1200 (amine)
AAS-M
Aminoethylaminopropyltrimethoxysilane
AO 700
AP 132
DAMO-P
DAMO-T
DC-Z 6020
Dow Corning Z 6020
Dynasylan DAMO
Dynasylan DAMO-P
Dynasylan DAMO-T
en-APTAS
G 91
G 91 (coupling agent)
Gelest SIA 0591.0
Geniosil GF 9
Geniosil GF 91
GF 91
HC 792
HD 107
Hydrosil 2776
JH 53
K 1600
KBM 603
KH 792
LS 2480
LS 3750
N-(beta.-Aminoethyl)-gamma.-aminopropyltrimethoxysilane
N-(.beta.-Aminoethyl)-3-aminopropyltrimethoxysilane
N-(2-Aminoethyl)-3-(trimethoxysilyl)propylamine
N-(2-Aminoethyl)-3-aminopropyltrimethoxysilane
N-(Aminoethyl)aminopropyltrimethoxysilane
N-(Trimethoxysilylpropyl)ethylenediamine

**Molecular Formula**
C8 H22 N2 O3 Si

2.1.3 **EC Number**
217-164-6

2.1.4 **CAS Number**
1760-24-3

2.1.5 **Other Identity Code**
None

2.2 **Structural Information**

2.2.1 **Structure and SMILES code**

\[
\text{NCCNCC[Si(OC)(OC)OC}
\]

2.2.2 **Optical Activity**
The substance is not optically active.

2.2.3 **Molecular weight**
222.36 g mol\(^{-1}\)
2.3 Composition of the Substance

2.3.1 % range of major constituent

>80%
Deviation below this purity value may be acceptable but should they occur a company should assess their statistical significance and submit new information if necessary.

2.3.2 Nature of Impurities

2.3.2.1 Listing of any impurities common to all suppliers
None

2.3.2.2 Description of the general structural types of other impurities
Hydrocarbon, aza-alkoxysilane and alkoxyxilane impurities have been identified.

2.3.2.3 Listing of possible SVHC impurities
None

2.3.2.4 Listing of other impurities that may contribute to the classification and labelling of the substance
None of the impurities contribute to the classification and labelling of the substance.
Specific details are given in the Confidential Annexes.

2.3.3 Percentage of Impurities

2.3.3.1 Information on impurities >1%
Four companies have disiloxanes present at >1%.

2.3.3.2 Information on SVHC >0.1%
None

2.3.4 Nature and Percentage of Any Additives
None
2.3.5 Spectral Data

2.3.5.1 NMR

Four companies have provided $^1$H and $^{13}$C NMR spectra. One company has provided a $^{29}$Si spectrum.

2.3.5.2 MS

Five companies have provided MS data.

2.3.5.3 IR

Five companies have provided IR spectral data.

2.3.5.4 UV

Not needed because the substance contains no known UV chromophores.

2.3.6 Chromatographic Data

2.3.6.1 GC

Five companies have provided GC data.

2.3.6.2 HPLC

Not needed as purity has been established by GC.

2.3.7 Analytical Methods

This report is based on analytical data provided by the member companies and reviewed by PFA. Individual companies are responsible for providing their own analytical data and appropriate method descriptions as part of their registration submission.
Confidential Annexes

These are found in report PFA.300.001.209A. For each company with an interest in the SIP, the annex contains a brief statement of what analytical data has been provided, the purity of the substance and the name and percentage of identified impurities. The confidential annexes will be made available to authorised representatives of the Reconsile Consortium and to the authorities as may be required.