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	ent No.: 00-S-RE-2012			<b>Rev.:</b> 02	Page: 1 of 153					
Classification Code: UNCLASSIFIED										
Origina	Originator: ACC Tag No.: NA System No. : 8600 Area Code: A101B									
SUPPORT ON INPUT TO ENVIRONMENTAL DISCHARGES – EVALUATION OF DEGRADATION COMPONENTS										
02	2010.08.24	IFC	HKL	KS	HKL					
01	2010.06.07	Issued for design	HKL	KS	HKL					
Rev.	Issue date	Description	Made b	y Chk. by	Appr. by					
<b>European CO<sub>2</sub> Technology Centre Mongstad (TCM)</b> This document contains proprietary and confidential information from Aker Clean Carbon										



		SINTEF REPC	RT		
	NTEF	TITLE			
SINTEF Materia	ls and Chemistry	TCM Amine Project: Support on input to e discharges	nvironmental		
NOR Location: Bratte 4. etg Telephone: +47.4	orkaia 17C,	Evaluation of degradation components Version 3			
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		CLIENT(S) Aker Clean Carbon ASA			
REPORT NO.	CLASSIFICATION	CLIENTS REF.			
SINTEF F16202	Confidential	Hans Konrad Lundekvam			
CLASS. THIS PAGE	ISBN	PROJECT NO.	NO. OF PAGES/APPENDICES		
Confidential		80134200	64 / 6		
ELECTRONIC FILE CODE		Odd Gunnar Brakstad			
FILE CODE	DATE	APPROVED BY (NAME, POSITION, SIGN.)	$\chi$		
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ABSTRACT

In this report potential degradation products relevant for TCM amines are described. The data presented here should be used as a background for the TCM Discharge permit application.

Possible degradation products are described for the post combustion process, including health and environmental data for the degradation products. The post combustion degradation products are described from experimental studies and were separated in 3 groups according to volatility; volatiles, medium volatiles and non-volatile products. In addition, degradation products from atmospheric processes are described, based on a theoretical study conducted by NILU. Theoretical degradation products from biological processes are predicted from a biodegradation/biocatalysis database.

Health- and environment (HE) data for degradation products were collected from several databases, including different HE-data sheets, the the International Uniform ChemicaL Information Database (IUCLID), the ECOTOX database of the US Environmental Protection Agency (EPA), the BIODEG database of the Syracuse Research Centre (SRC), and the GENE-TOX database (EPA).

This data search showed that the available HE information from amine degradation products are not complete for performing proper risk assessment, and further data should be obtained to fill the gaps, either from confidential literature or from experimental studies. Before any solvent is tested at the CO<sub>2</sub> technology centre, solvent degradation and emissions will be studied in lab-scale, a SINTEF lab-scale pilot, SINTEF's full height pilot-plant at Tiller (Trondheim) and ACC's Mobile Test Unit.

A specific search for health-related effects were performed for potential amine degradation products (nitrosamines, nitramines and amines/amides) of 5 relevant TCM solvents. The search showed that all amine degradation products must be considered as a possible environmental health hazard. Provisional permissible air limits based on occupational exposure limits indicated that ntrosamines may contribute to the health risk of the population even if there emission concentrations are small. However, no ground level concentrations of these products have not yet been estimated, and their real risks are therefore not yet known.

A search for pre-registration in REACH showed that most of the products were pre-registered.

KEYWORDS	ENGLISH	NORWEGIAN
GROUP 1	Environment/Health	Miljø/Helse
GROUP 2	Absorption	Absorpsjon
SELECTED BY AUTHOR	CO <sub>2</sub> capture	CO <sub>2</sub> fangst
	Amines	Aminer
	Degradation products	Degraderingsprodukter

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### ABBREVIATIONS

bw - Body weight

- CPDB Carcinogenic Potency Project Database
- DNEL Derived No-Effect Level
- EC European Community
- EC<sub>50</sub> Effective Concentration causing 50 % inhibition of growth for a population of uniform organism
- EIA Environmental Impact Assessment
- EPA U.S. Environmental Protection Agency
- EU European Union

GESAMP - IMO/FAO/UNESCO/IOC/WMO/WHO/IAEA/UN/UNEP Joint Group of Experts on

the Scientific Aspects of Marine Environmental Protection, 2002. Revised GESAMP Hazard

Evaluation Procedure for Chemical Substances Carried by Ships

- HE Health and Environment Information about a substance
- IRIS Integrated Risk Information System
- IUCLID International Uniform Chemical Information Database
- $LC_{50}$  Concentration causing 50 % lethality for a population of uniform organism
- $LD_{50}$  Lethal dose causing 50 % lethality for a population of animals
- MTU Mobile Test Unit
- MSDS Material Safety Data Sheets
- NILU Norwegian Institute of Air Research
- NOEC No-effect concentrations (effect limit in ecotoxicity tests)
- NOAEL No-observed adverse effect limit (effect limit in toxicity tests related to human health)
- OECD Organisation for Economic Cooperation and Development
- OEL Occupational Exposure Limit
- PNEC Predicted No-Effect Concentration
- REACH European Regulation for Registration, Evaluation, Authorisation and restriction of Chemicals
- RTECS Toxic Effects on Chemical Substances®: Number indicate record number
- SMILES Simplified Molecular Input Line Entry Specification
- SRC Syracuse Research Company
- TCM Technology Centre Mongstad
- TGD Technical Guidance Document
- UM-BBD The Biodegradation and Biocatalysis Database at the University of Minnesota

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### **Executive Summary**

In this report potential degradation products relevant for TCM amines are described, as well as the health and environmental hazard related to emissions of these products. The data presented here should be used as a background for the TCM Discharge permit application.

An extensive review has been carried out of reported degradation products of the solvents used in the  $CO_2$  capture process, mainly from open scientific literature. In addition, a lot of work on identification of degradation products is going on in the SOLVit project, including development and use of analytical tools for identification and quantification of solvent degradation products.

The computational chemistry model SM8 has been used for separation the degradation products in three categories; volatile, medium volatile and non-volatile degradation products. It is expected that the water wash will be less efficient for capturing volatile products, while emissions of medium volatile products with vapour pressure comparable to the amine solvents will be low. Non-volatile products are expected to have significant vapour pressure and are expected to be emitted to a significant degree through entrainment. In the report a number of classes of degradation products are listed, including open chain molecules with amine, amide, alcohol, carboxylic acids, and 5 classes of cyclic compounds.

There are two main forms of solvent degradation; oxidative degradation and thermal degradation. In addition, degradation may be caused by SOx and NOx. Most solvent degradation involves cleavage and formation of N-C and O-C bonds. Thermal degradation is mainly believed to be the degradation of the carbamate form of the solvent, and the main mechanisms well understood, while the mechanisms of oxidative degradation are not yet established.

MEA degradation has been studied to some extent, although there still exists a number of unidentified degradation products from this amine. For some of the other possible TCM solvents there is limited experimental data available. Before any solvent is tested at the CO2 Technology centre, solvent degradation and emissions will be studied in lab-scale, a SINTEF lab-scale pilot, SINTEF's full height pilot plant at Tiller (Trondheim) and ACC's mobile test unit (MTU).

In the present report we summarize degradation products for the different TCM solvents, mainly based on MEA degradation. However, degradation products specific to other TCM solvents have also been included. The information is mainly based on experimentally observed degradation products, but we have also included some degradation products that may be expected to form, but that have still not been identified in experimental work. Each solvent forms a significant number of degradation products (in some cases more than 50), and identification of degradation products have not been completed for some solvents.

A number of 18 volatile degradation products are described in the report. Emission concentrations of these products are difficult to predict, but we have estimated emission of individual volatile products relative to ammonia emission, since ammonia emissions are a good indicator of the overall extent of degradation in a CO<sub>2</sub> capture plant. We believe that most formation of volatile degradation products is due to oxidative degradation, since this is the form of degradation that is believed to dominate in a post-combustion CO<sub>2</sub> capture plant. A number of 9 possible medium volatile degradation products were identified, although this list is far from complete, and if these represent the most important HE-relevant products has not been established. For each solvent



there may perhaps be 10-50 degradation products that fall in this category. The non-volatile degradation products are mainly organic acids, and 4 acids were listed in the report.

Some of the degradation products are of special concern due to their health risks, with main focus on nitrosamines and nitramines. And a separate list was therefore prepared for possible nitrosamines. Nitrosamine and nitramines are formed as a result of reactions between NOx components and amine species. The formation of nitrosamines are mainly associated with secondary amines, but may be formed also from systems with primary and tertiary amines. Nitrosamines have been detected also in measurement campaigns. At present we are not aware that any dedicated work has been done to identify nitramines in degraded amine solvents.

The emission of a given degradation product depends on concentration of the component, the compounds chemical properties, the design of the capture plant and in particular the water-wash section. The water wash will be most efficient for medium volatility and non volatile degradation products, while an acid wash should be efficient in reducing emissions of any compounds that have base strength, like ammonia, alkylamines, solvent components and degradation products with amine functionalities. The effect of an acid-wash on nitrosamine emissions is hard to predict and is an issue that should be studied further. Many medium volatility and non volatile degradation products are likely to be present in concentrations that are less than 1% of the solvent concentration, and several of the products are less volatile than the amine itself.

Further work is required to determine the emissions of nitrosamines and nitramines, and it would be advantageous to have a group detection method for these compounds.

In our view this sampling should be carried out both of the emissions from the plant and the exhaust gas coming into the plant. LC-MS scan analysis of liquid samples from the water-wash can be used to check if there are any unexpected degradation products being emitted to a significant degree.

Degradation of solvents after emissions to air is mainly the result of photochemical processes, and a theoretical study of this has been performed by NILU. In addition both solvents and degradation products are subject to biological degradation in biotic environments. Experimental and theoretical studies of amine biodegradation results in deamination with a number of aldehydes, alcohols and organic acids as putative products.

The potential health and environmental effects of identified TCM solvent degradation products were investigated by obtaining information from the several databases, (IUCLID, ECOTOX, IRIS og GENE-TOX, Toxnet, GESAMP, CPDB, and the BIODEG database of the Syracuse Research Centre) and from material safety data sheets of individual degradation products. The environmental impacts were investigated for three trophical levels of aquatic organisms and biodegradability. Health related information was collected for endpoints recommended in REACH, including acute toxicity, mutagenicity/genotoxicity, reproduction toxicity, irritation/corrosion, sensitization and repeated dose toxicity.

Data from ecotoxicity information varied considerable, reflecting different toxicity levels, but also that tests have been performed by different laboratories, by different methods, and with different species within each trophic level (fish and algal species). Variations between tests were higher for volatile than for medium and non-volatile products. The combination of expected low emission, water-solubility (low bioaccumulation potentials), biodegradability and low to moderate acute ecotoxicity for most of the post combustion degradation products, indicate that the environmental risk associated with these products should be moderate or low. However, some of the degradation



products may persist in the environment due to poor biodegradability, and this may pose a possible risk if accumulated in the environment. Nitrate may be formed by biological oxidation of ammonia, and high input of ammonia may therefore result in increased fertilization effects in the local catchment area, although this will require very high ammonia emissions. The data search showed that environmental information for possible nitrosamines was limited.

Health hazards were associated with several of the degradation products. Although some of the degradation products are well known chemicals, essential health-related data for several of the products were not available in the searched databases. The acute toxicity varied considerable between the products, but also for the same product, questioning the quality of several of the tests performed. Mutagenic and genotoxic effects are well documented for the nitrosamines, but were also found for volatile aldehydes and alkylamines. Several of the products lacked data for reproduction toxicity, and for both this endpoint and for repeated dose toxicity there is a lack of standardization for result presentation, which complicates interpretation and comparison of the results. Most of the degradation products were corrosive and/or irritating, while only a few showed sensitizing characteristics. Data for degradation products pre-registered in REACH will be available from vendors after REACH registration.

Based on the environmental data PNEC values may be calculated for most of the degradation products, while DNEL could only be calculated for a few products.

A number of 27 degradation products from 5 TCM-relevant solvents were selected for closer health-related examination. These represented only N-compounds, including nitrosamines, nitramines and amines/amides. Several databases were used for obtaining data on human health hazard. Toxicity was grouped in oral, dermal, and inhalation toxicity, as well as long-term toxicity, the latter defined as carcinogenic, mutagenic and reproduction effects. For each endpoint a rating was given. In additional occupational exposure levels (OEL) were described.

A first provisional risk evaluation of the 27 degradation products were conducted, with an OEL divided by 100 to represent a permissable exposure limit for the general population. This resulted in ambient air limits of 0.01 to  $180 \ \mu g/m^3$ , with nitrosamines, nitramines and amines converted to nitrosamines with the lowest limits. Based on these limits nitrosamines may contribute to the health risk of the population, although their emission concentration is small. However, the real risks can no be estimated before the fate of these compounds have been determined.

It was shown that most of the 27 degradation products were pre-registered in REACH, meaning that improved HE-information for these will be available in near future.



### **Overordnet sammendrag**

I denne rapporten beskrives mulige degraderingsprodukter som er relevante for TCM aminer, samt iboende helse- og miljørisiko knyttet til utslipp av dem. Dataene presentert her skal kunne brukes som en bakgrunn for søknad om utslippstillatelse fra TCM.

En gjennomgang har blitt utført av rapporterte degraderingsprodukter fra solventer brukt i CO<sub>2</sub>fangst prosesser, hovedsakelig fra vitenskapelig litteratur. I tillegg utføres det et betydelig arbeid med å identifisere degraderingsprodukter gjennom SOLVit prosjektet, bl.a. utvikling av analytiske verktøy for identifisering og kvantifisering av solvent degraderingsprodukter.

Beregningsverktøyet SM8 for kjemimodellering har blitt brukt for separering av degraderingsproduktene i tre kategorier; flyktige, medium flyktige og ikke-flyktige produkter. Det er forventet av vannvask vil være mindre effektiv for oppfanging av flyktige produkter, mens utslipp av medium flyktige forbindelser med damptrykk sammenlignbart med amin-solventen vil være lav. Ikke-flyktige produkter er forventet å ha betydelig damptrykk, og derfor er det sannsynlig at disse slippes ut i betydelig grad ved medrivning. I denne rapporten er et antall klasser av degraderingsprodukter opplistet, bl.a. 5 klasser av sykliske forbindelser, og åpen kjede molekyler som aminer, amider, alkoholer og karboksylsyrer.

Det er to former for solvent degardering; oksydativ og termisk degradering. I tillegg kan degradering forårsakes av SOx og NOx. De fleste mekaniser for solvent degradering inkluderer kløyving og dannelse av N-C og O-C bindinger. Termisk degradering er antatt å være degradering av karbamat-formen av solventen, og mekanismen er godt beskrevet, mens mekanismer for oksydativ degradering ikke er etablert ennå.

MEA degradering er relativt godt studert, men fremdeles eksisterer et antall uidentifiserte degraderingsprodukter fra dette aminet. For noen av de andre alternative TCM solventene er kun et begrenset antall data tilgjengelige fra eksperimentelle studier. Før solventer testes ved CO2 teknologisenteret på Mongstad vil degradering og utslipp bli studert i labskala, en SINTEF labskala pilot, ved SINTEFs fullskala pilotanlegg på Tiller (Trondheim) og ved ACCS sine mobile testenhet (MTU).

I denne rapporten oppsummeres degraderingsprodukter fra de ulike TCM-solvents, hovedsakelig basert på MEA degradering. Imidlertid har degraderingsprodukter basert på andre TCM solvents også blitt inkludert. Informasjonen er hovedsakelig basert på eksperimentelt observerte degraderingsprodukter, men vi har også inkludert noe degraderingsprodukter som kan forventes å dannes, men som ikke har blitt identifisert eksperimentelt. Hver solvent kan danne et betydelig antall degraderingsprodukter (i noen tilfeller mer enn 50), og identifikasjon av produktene er ennå ikke fullført for alle solventene

Atten flyktige degraderingsprodukter er beskrevet i rapporten. Utslippskonsentrasjonene for disse produktene er vanskelige å anslå, men vi har estimert utslipp av enkeltprodukter sammenlignet med utslipp av ammoniakk, siden ammoniakk-utslipp er en god indikator på graden av degradering i et CO<sub>2</sub>-fangst anlegg. Vi antar at det meste av dannelsen av flyktige degraderingsprodukter skyldes oksydativ degradering, siden dette er den formen for degradering som forventes å dominere i et etterforbrennings CO<sub>2</sub>-fangst anlegg. Ni mulige medium flyktige degraderingsprodukter ble identifisert, men denne listen er mangelfull, og det er usikkert om disse representerer de viktigste produktene med tanke på helse og miljø. Det er forventet av hver



solvent kan gi opphav til 10-50 degraderingsprodukter fra denne kategorien. Ikke-flyktige degraderingsprodukter er hovedsakelig organiske syrer, og 4 slike syrer er opplistet i rapporten.

Noen av degraderingdsproduktene er knyttet til spesiell helserisiko, spesielt nitrosaminer og nitraminer. En egen liste er derfor laget for identifisering av mulige nitrosaminer. Nitrosaminer og nitraminer dannes ved reaksjon mellom NOx komponenter og aminer. Dannelsen av nitrosaminer er hovedsakelig forbundet med sekundære aminer, men kan også dannes fra systemer med primære og tertiære aminer. Nitrosaminer har blitt påvist i målekampanjer, men på det nåværende tidspunkt er vi ikke kjent med arbeid for å påvise nitraminer i degraderte amin solventer.

Utslipp av et gitt degraderingsprodukt avhenger av konsentrasjonen av komponenten, dens kjemiske egenskaper og design av fangstanlegget, spesielt vannvask-seksjonen. Vannvasken vil være mest effektiv for medium flyktige og ikke-flyktige degraderingsprodukter, mens syrevask vil være effektiv i å redusere utslipp av alle basiske komponenter, f.eks. ammoniakk, alkylaminer, solvent-komponenter og degraderingsprodukter med amin-funksjonalitet. Effekten av syrevask på nitrosaminer er vanskelig å anta og bør derfor studeres videre. Mange medium flyktige og ikke-flyktige degraderingsprodukter er antatt å forekomme i konsentrasjoner mindre enn 1 % av solventens konsentrasjon, og flere av produktene er mindre flyktige enn selve aminet.

Videre studier er påkrevd for å bestemme utslipp av nitrosaminer og nitraminer, med det vil være fordelaktig med en gruppe-basert deteksjonsmetode for disse forbindelsene. Vårt syn er at prøvetaking kan utføres både på utslipp fra anlegget og eksosgassen som kommer inn i anlegget. LC-MS scan analyser av væskeprøver fra vannvask kan brukes for å undersøke om uventede degraderingsprodukter slippes ut i betydelig grad.

Degradering av solventer etter utslipp til luft er hovedsakelig et resultat av fotokjemiske prosesser, og en teoretisk studie av dette har blitt utført av NILU. I tillegg vil både solventer og degraderingsprodukter kunne biodegraderes i biotisk miljø. Eksperimentelle og teoretiske studier av amin biodegradering resulterer i deaminering med dannelse av aldehyder, alkoholer og organiske syrer som mulige produkter.

De potensielle helse- og miljøeffekter av identifiserte degraderingsprodukter fra TCM solventer ble identifisert med informasjon fra flere databaser (IUCLID, ECOTOX, IRIS og GENE-TOX, Toxnet, GESAMP, CPDB, og BIODEG databasen fra Syracuse Research Centre) og fra HMS datablad for individuelle degraderingsprodukter. Miljøeffekter ble vurdert for vannorganismer som representerer tre trofiske nivåer. Helserelatert informasjon ble innsamlet for endepunkter anbefalt av REACH; akutt giftighet, mutagenitet/genotoksisitet, reproduksjonsgiftighet, irritasjon/etsing, allergi og kronisk toksisitet ved gjentatt dosering.

Økotoksikologiske data varierte betydelig. Dette kunne skyldes varierende toksisitetsnivåer, men også at tester har blitt utført av ulike laboratorier, med ulike metoder, og med forskjellig dyrearter på hvert trofisk nivå (fisk- og algearter). Variasjoner mellom tester var høyere for flyktige komponenter enn medium flyktige og ikke-flyktige forbindelser. Kombinasjonen av forventet lave utslipp, vannløselighet (lavt bioakkumuleringspotensiale), biodegraderbarhet og lav eller moderat økotoksisitet for de fleste degraderingsproduktene, indikerer at miljørisikoen assosiert med disse forbindelsen vil være moderat til lav. Imidlertid bør man være oppmerksom på noen av degraderingsproduktene er lite biodegraderbare, noe som kan gi en mulighet for at de kan akkumulere i miljøet. Nitrat kan dessuten dannes ved biologisk oksydasjon av ammoniakk, og dannelse av nitrat kan gi øket næringstilgang i lokalt nedbørsfelt. Dette vil imidlertid kreve



betydelig utslipp av ammoniakk. Datasøk viste at miljøinformasjon for mulige nitrosaminer var begrenset.

Det ble vurdert mulig helserisiko for flere av produktene. Imidlertid var det begrenset helseinformasjon tilgjengelig for mange av produktene, selv om mange av disse var relativt velkjente kjemikalier. Akutt giftighet varierte betydelig mellom produktene, men også mellom tester utført på samme kjemikalium, noe som setter et spørsmålstegn med kvaliteten på utførelsene av flere av testene. Mutagene og genotoksiske effekter er godt dokumenter for nitrosaminer, men ble også påvist for flere av de flyktige aldehydene og alkylaminene. Mange av degraderingsproduktene manglet data for reproduksjonsgiftighet, og både for dette endepunktet og for kronisk toksisitet med gjentatt dosering mangler en entydig standardisering av presentasjonen av dataene. De fleste produktene var etsende og/eller irriterende, mens kun et fåtall var potensielt allergiframkallende. Data for degradatingsprodukter pre-registrert i REACH vil bli tilgjengelige fra leverandører etter registrering.

Basert på miljødata ble PNEC verdier beregnet for de fleste produktene, mens DNEL kun ble beregnet for et fåtall produkter pga. mangel på relevante data.

Et antall på 27 degraderingsprodukter fra 4 TCM-relevante solventer ble utvalgt for en nærmere helse-basert vurdering. Disse representerte N-forbindelser som nitrosaminer, nitraminer og aminer/amider. Flere databaser ble benyttet for å framskaffe helserelaterte data. Toksisitet ble gruppert i oral, dermal og inhalasjonstoksisitet. Langtids toksisitet ble definert som karsinogen, mutagen og reproduksjons-effekter. Hvert endepunkt ble gitt en rangering.

En første midlertidig risokoevaluering av de 27 degraderingsproduktene ble utført, med en OEL dividert på 100 for å representere en tillatelig eksponeringsgrense for den generelle befolkningen. Dette resulterte i grenserverdier for luft på 0.01 til 180  $\mu$ g/m<sup>3</sup>, med nitrosaminer, nitraminer og aminer omdannet til nitrosaminer med de laveste grenseverdiene. Disse grenseverdiene viser at nitrosaminer kan bidra til helserisiko for den generelle befolkningen, selv om utslippskonsentrasjonene er små. De reelle risiko-vurderinger kan imidlertid ikke utføres før beregninger av degraderingsproduktenes skjebne er utført.

Det ble også vist at de fleste av de 27 degraderingsproduktene var pre-registrert i REACH, dvs. at forbedret HM-informasjon vil bli tilgjengelig i nær framtid.

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### 1 Background

The objective of the project was to improve documentation of potential health and environmental impacts of amine solvent emissions from the CO<sub>2</sub> Technology Centre at Mongstad (TCM). This information will serve as input to the Discharge permit application for TCM. This documentation includes a) quality assurance (QA) of information on health and environment (HE) provided by the suppliers of selected solvents relevant for TCM, b) evaluations of solvent degradation products emitted to the environment and generated in the environment after emission, c) evaluation of environmental effects of some expected degradation products.

Several relevant solvents and solvent mixtures were evaluated. Monoethanolamine (MEA) was used as a base case in this project, since MEA will be used as amine solvent during the initial phase of the TCM operation.

Specific issues described in this report include:

- Evaluation of design values for amine emissions control when operating an absorber with two water wash stages for base case and alternative solvents
- Identification of degradation products from relevant TCM solvents, based on experimental data from relevant literature studies
- Comparison of literature data to updated information from new emissions measurement campaigns (Longannet, Scotland, Summer 2009)
- Update HE information on the degradation products, based on experimental and theoretical data
- Specific health-reletaed information for amine-based degradation products relevant for selected TCM solvents

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### 2 Amine degradation products

Degradation of amines may appear in three different compartments, a) reaction products in the post combustion process, b) after emission to air, and c) after emission to soil or aquatic environments. It is difficult to predict which compartment will be most important from a health and environmental perspective, since the fate of amines and degradation products are yet not well elucidated in each compartment. Complex processes may take place in all the compartments. The risk of generation of hazardous degradation products (e.g. nitrosamines and nitramines) are generally associated with the air compartment, but soil and water compartments may be important for depletion of these compounds through biological transformation processes. The emphasis of this study has been put on characterisation of the reaction products from the post combustion process and available HE-data for these products.

### 2.1 Degradation products in the post combustion process

### 2.1.1 Background

An extensive review has been carried out of reported degradation products of the solvents used in the CO<sub>2</sub> capture process. The main sources have been work by Axel Meisen and co-workers, Gary Rochelle and co-workers and work at the DOW chemical company (Davis and Rochelle, 2008; Sexton and Rochelle, 2008). We have also drawn on the PhD thesis of Helene Lepaumier and a paper by Strazisar and co-workers (Lapaumier, 2008; Strazisar et al., 2006; Strazisar et al., 2003). Furthermore, as a part of the SOLVit project we also have considerable ongoing research into solvent degradation. As part of this work we have observed many of the same species as reported in the literature.

It should be noted that conclusive identification of degradation products can be technically challenging. Reports of degradation products reported in the open scientific literature must therefore also be treated with a certain caution; this is especially the case with degradation products that have only been observed by a single research group.

In addition to the literature in the field of post-combustion  $CO_2$  capture, there is the broader research literature on amine chemistry and nitrosamine chemistry. An example is the review of nitrosamine chemistry edited by Loeppky and Michejda (1994). While this literature contains much chemistry that is of relevance to solvent degradation, caution must be taken in extrapolating results from this literature to solvent degradation in  $CO_2$  capture plants. The extent to which chemical reactions take place depends on conditions such as temperature, pH and concentration of different components. Reactions that are dominant in one set of conditions, may play a negligible role under other conditions.

### 2.1.2 Work on Solvent Degradation in SOLVit

In the SOLVit project there is extensive ongoing work to understand solvent degradation and emissions from  $CO_2$  capture plants. Solvent degradation is studied both in bench-scale experiments and pilot plants. Before any solvent is tested at the European  $CO_2$  technology center, solvent degradation and emissions will have been studied in lab-scale, a SINTEF lab-scale pilot, SINTEF's full hight pilot-plant at Tiller (Trondheim) and ACC's Mobile Test Unit.



The work on solvent degradation is focused on identification of any components that may present HSE issues or affect the efficient operation of the CO<sub>2</sub> capture process.

A dedicated method has been developed for the detection and quantification of nitrosamines. This is being applied to quantify nitrosamine formation in pilot plants.

The main analytical tools used for identification of degradation products in SOLVit is LC-MS, GC-MS and Ion-Chromatography (IC). A LC-MS scan technique is used to give a qualitative picture of degradation products formed. The scan technique can pick up most ionisable degradation products with molecular weight higher than 70. From the scans the molecular weight of the degradation products is obtained. Further analytical work is however required to identify and quantify each degradation product. For lighter components scan techniques are less reliable, for such components the analytical methods must be tuned to search for specific components.

We believe that we in SINTEF are capable of detecting most components formed in solvent degradation, and we have an ongoing process to close remaining gaps in detection of degradation products. Before any solvent enters TCM we should be able to identify all components that form a significant part of the emissions from the plant.

Analytical work is ongoing for a number of solvents. We believe we have detected most degradation products for a number of solvents being developed in SOLVit. The types of components formed are also in most cases known. The molecular weight and gross molecular weight of the degradation products are in many cases known, but there are in many cases uncertainty regarding the exact molecular structure.

### 2.1.3 Assessment of the Literature on Solvent Degradation

There is a substantial body of literature on solvent degradation. Much of this is however focused on thermal degradation of solvents. Thermal degradation is the type of degradation most relevant to acid gas removal from natural gas. For this form of degradation the main reaction mechanisms and likely degradation products appear to be fairly well understood.

It is only in recent years that substantial research has been published on oxidative degradation; the form of degradation that would appear to be most relevant to post-combustion  $CO_2$  capture.

For oxidative degradation a number of degradation products are known, the mechanistic details of oxidative degradation are however to a large extent uncertain.

Much of the literature on oxidative degradation is based on lab-scale experiments. The conditions in these experiments do often deviate substantially from those encountered in a  $CO_2$  capture plant. One should therefore be careful in extrapolating from such studies to pilot plants. Lab-scale experiments may both overstate and understate the formation of degradation products.

A lot of the analytical work on solvent degradation in the literature is based on IC and GC-MS techniques. While we believe these techniques are well suited to identification of a number of key degradation products, there are likely to be components that can not easily be identified with these techniques.

The degradation work carried out in SOLVit with LC-MS techniques suggests that there are heavier components formed that have not been reported in the literature.



The research published in the open scientific literature on solvent degradation has historically been mainly focused on understanding and quantifying degradation. Health and environmental aspects of solvent emissions have until recently been less of a concern in most work on solvent degradation. This means that there has been more focus on identifying main degradation products, rather than looking for components that may present health and environmental issues.

Finally, it should be noted that identification and quantification of solvent degradation products in some cases may involve quite demanding analytical chemistry. Some degradation products may be chemicals that have not previously been studied or synthesized. In such a case confident identification will require a number of steps.

### 2.1.4 Volatility

We have used the computational chemistry model SM8 (Solvent Model 8, Marenich et al. 2007) to calculate the free energy of solvation of different degradation products and looked at which components are likely to be present in ionic form under process conditions. Based on these results we have separated the degradation products into three categories: volatile degradation products, medium volatility (with volatility comparable to the amine solvents) degradation products and nonvolatile degradation products. Non-volatile degradation products are components that are on ionic form in post-combsution  $CO_2$  capture conditions (such as organic acids). Medium volatility degradation products are defined as other degradation products that have volatility comparable to, or lower, than 2-ethanolamine (MEA). Volatile degradation products are components with higher volatility than MEA.

The relationship between the free energy of solvation and the vapour pressure of the species is given by the following equation (Winget et al. 2000):

$$P_{vapor,j} = \frac{RT}{\rho} \frac{x_j}{\sum_i x_i M_i} \exp\left(\frac{\Delta G_{solv}}{RT}\right)$$
(2.1)

 $x_j$  is the mole fraction in the liquid phase of the component in question. *M* is the molar mass,  $\rho$  is the density, *T* is the temperature and R is the universal gas constant.

The free energy of solvation of MEA is predicted to be -9.0 [kcal/mol] by the SM8 model, a lower free energy of solvation indicates that a component is less volatile than MEA.

It can be noted that the vapour pressure is a function of the concentration of a species and it's free energy of solvation (volatility). To predict the emissions of a given component, we need to know both the concentration of a species and the free energy of solvation. The free energy of solvation can be calculated with a high degree of confidence, and the main uncertainty is the concentration of a component in the  $CO_2$  capture plant.

Volatile degradation products will tend to evaporate to a significant degree and follow the exhaust gas out of the absorber. The water-wash will also be less efficient in capturing volatile degradation products.

Medium volatility degradation products have vapour pressure comparable to the amine components. Their concentration will however tend to be orders of magnitude lower than for the solvent itself. The emission level is therefore likely to be low.



Non-volatile degradation products are species that are either in ionic form in the absorption liquid or are both heavy and hydrophile. These are not expected to have any significant vapour pressure. They would only be expected to be emitted in a significant degree through entrainment.

### 2.1.5 Type of components formed

Degradation products can be classified by their chemical structure and functionality. In Table 2.1 we have listed examples of all classes of degradation products that we are aware of. All degradation products from TCM solvents are expected to fall within these categories.

We have identified 5 different classes of cyclic compounds. Other degradation products are open chain molecules with amine, amide, alcohol and/or carboxylic acid functionalities.

Nitrosamines and nitramines are classes of degradation products that may be important from a health and environmental risk perspective, even if their rate of formation is low.

Class/Degradation product	CAS.	Structure	Ref./Comment
Oxazolidine	497-25-6		Observed in pilot-plants. Certain degradation product in MEA. Some other TCM solvents are expected to form analogues (with subsituent groups on the carbon chain and amine functionality)
Imidazolidinone 1-(2_hydroxyethyl)-2- imidazolidinone (HEIA)	3699-54- 5	HO HO	Observed in pilot-plants. Certain degradation product in MEA.
Imidazole N-(2-hydroxyethyl)imidazole (HEI)	1615-14- 1	OH N	Observed in pilot-plants. Observed in MEA (work of Andrew Sexton and NTNU/SINTEF).
Piperazine and piperazine derivatives	110-85-0	HNNH	Not expected to form to significant degree in MEA. Likely to be significant for TCM solvent 9. Substituted piperazines may also form.
Morpholine	110-91-8	O	May form to limited extent in MEA and other TCM solvents.
Open chain amine/alcohol N-(2-hydroxyethyl)- ethylenediamine, HEED	111-41-1	HO NH <sub>2</sub> H	Observed in pilot-plants. Certain degradation product in MEA.

#### **Table2.1** Types of degradation products



### Table2.1 Continued

Class/Degradation product	CAS.	Structure	Ref./Comment
<u>Alkylamine</u> Methylamine	74-89-5	H <sub>2</sub> N	Has been observed in MEA in recent solvent degradation research by Statoil (Pedersen et al. 2010)
Organic acid Oxalic acid	144-62-7	но он	Observed in pilot-plants. Certain degradation product in MEA. Expected in most solvents.
<u>Open chain amides</u> N-(2-hydroxyethyl)- Formamide (HEF)	693-06-1	HO	Observed in pilot-plants. Certain degradation product in MEA. Similar degradation products expected in most solvents.
<u>Nitrosamines</u> 4-nitroso-morpholine	59-89-2		Observed in ACCs Longannet Campaign. Some degree of formation of nitrosamines appears likely in most solvents.
<u>Nitramines</u> Dimethylnitramine	4164-28- 7		Not observed in context CO <sub>2</sub> capture solvents. To our knowledge no dedicated analytical method is at presently available. Some degree of formation appears likely.

### 2.1.6 Degradation mechanisms

There are two main forms of solvent degradation: oxidative degradation and thermal degradation. In addition there is degradation caused by SOx and NOx. Other impurities in the exhaust gas such as fly ash may also contribute to solvent degradation.

Oxidative degradation is expected to be the main form of degradation in post-combustion  $CO_2$  capture.

Some main observations can be made based on what we know about solvent degradation chemistry. Most solvent degradation involves cleavage and formation of N-C and O-C bonds. There also appears to be some degradation mechanisms involving cleavage of C-C bonds, the extent of degradation involving C-C bond formation appears to be very limited. There is also clear evidence of reactions involving both ring formation and ring opening.

Degradation proceeds through a number of reaction steps, while some degradation products are stable and accumulate over time, many will undergo further reactions. This also means that over time thermal degradation products can react with oxidative degradation.

In a  $CO_2$  capture plant we observe the formation of degradation products, but associating the observed degradation in a plant to a specific form of degradation is difficult.



Thermal degradation is mainly believed to be degradation of the carbamate form of the solvents. The main mechanisms for thermal degradation we believe are well understood. For oxidative degradation the mechanisms are however not established. There has to our knowledge been few experimental studies of degradation by SOx, NOx and other impurities.

As degradation proceeds there is an accumulation of heavier degradation products.

### 2.1.7 State of knowledge on different solvents

2-ethanolamine (MEA) is one of the solvents for which degradation has been studied the most extensively. Even for this solvent there are however still some unidentified degradation products. The degree of formation of different degradation products in a  $CO_2$  capture plant has also not been fully quantified yet. Many of the unidentified degradation products are however low-volatility heavier compounds that are not expected to be emitted to a significant degree (probably concentrations at ppb level or lower).

For some of the other possible TCM solvents there is limited experimental data on solvent degradation. There is ongoing testing of these solvents in the SOLVit project but identification of degradation products is still ongoing. For several solvents we therefore rely on assumptions of similar patterns in degradation as seen for MEA or other solvents where experimental data are available.

All degradation products that we are aware of fall within the classes of compounds given in Table 2.1. We also expect that most, if not all, unknown degradation products fall within these groups.

As described in section 2.1.2 all solvents that go into use at TCM will be tested in pilot-plants. As a part of pilot-plant campaigns there will be extensive testing of solvent degradation and emissions and more information will be available before start-up of TCM.

### 2.1.8 Observed and Proposed degradation products

In the present chapter we summarize degradation products for the different TCM solvents. We have chosen to present a joint set of tables for the TCM solvents. The tables are intended to give a representative view of degradation products formed.

This summary is mainly based on MEA degradation, but degradation products specific to other TCM solvents have also been included. In the cases where a degradation product is specific to one or more TCM solvent this is indicated in the tables.

The tables are mainly based on experimentally observed degradation products, but we have also included some degradation products that may be expected to form, but that have still not been identified in experimental work.

There are several reasons for presenting a joint set of tables, rather then separate sets of tables for each TCM solvent.

We do in general expect the same degradation mechanisms to be dominant for the different solvents. This means that in many cases degradation products will be the same or structurally similar.



Each solvent forms a significant number of degradation products (in some cases more than 50), and identification of degradation products have not been completed for some solvents. Another reason for presenting a single set of tables is to maintain the confidentiality regarding the solvents that will be tested at TCM. There are separate tables for volatile degradation products (Table 2.2), medium volatility degradation products (Table 2.3), non-volatile degradation products (Table 2.4) and nitrosamines (Table 2.5).

In preparing this work we have drawn on reports of emissions from the Esbjerg  $CO_2$  capture plant (da Silva and Aas 2010) and Eurofins measurement campaign at ACCs  $CO_2$  capture plant (Rokkjær and Vang 2009). We have also drawn on ongoing work in the SOLVit project.

We believe that the list of volatile degradation products in Table 2.2 is fairly exhaustive. In the table we have indicated an estimated emission of each component relative to the ammonia emission. The rationale for this is that we believe that ammonia emissions are a good indicator of the overall extent of degradation in a  $CO_2$  capture plant. We then assume that the extent of formation of volatile degradation products is proportional to the overall extent of degradation. In estimating the relative emissions we have drawn on available experimental emissions data and general knowledge of solvent degradation. These values assume water wash operation similar to what has been used in the Esbjerg  $CO_2$  capture plant.

It must be noted that there is still limited experimental data on formation of some of these volatile degradation products, and further work will be done prior to start-up of TCM to produce more confident estimates of emissions. Predicting the emissions of volatile degradation products can also be challenging since they can be a significant part of the emissions even if they are formed in very small amounts. There is therefore at present a need for emission measurements for these species.

We believe the likelihood of forming cyclic alkylamines such as pyrrolidine is quite low, since that would require a longer-carbon backbone than we encounter in most degradation products.

We believe that most formation of volatile degradation products is due to oxidative degradation, since this is the form of degradation that is believed to dominate in a post-combustion  $CO_2$  capture plant. The mechanistic details of the formation of these species is however not known, there are a number of impurities that may contribute to the formation of such degradation products.

Nitrosamines are listed in Table 2.5. Many of these are however also volatile degradation products.

The volatile degradation products are likely to evaporate from the liquid phase rapidly, they are therefore likely to be terminal degradation products (not undergoing further degradation in a  $CO_2$  capture plant).

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	C + C	B #14/	<u> </u>		
Degradation product	CAS.	MW	Structure	Relative conc.	Ref./Comment
Ammonia	7664-41-7	17.03	NH <sub>3</sub>	1	Certain degradation product in MEA. Likely to form in significant degree in most solvents.
Formaldehyde	50-00-0	30.03	Р	0.05	Certain degradation product in MEA. Likely to form to some degree in most solvents.
Acetaldehyde	75-07-0	44.05		0.05	Certain degradation product in MEA. Likely to form to some degree in most solvents.
Acetone	67-64-1	58.08		0.05	Observed in CASTOR. Surprising degradation product, may be impurity.
Formamide	75-12-7	45.04	0 NH2	0.1	Observed in laboratory experiments on degradation ( work of Andrew Sexton).
Methylamine	74-89-5	31.06	H <sub>2</sub> N	0.01	Has been observed in MEA in recent work by Statoil (Pedersen et al. 2010).
Acetamide	60-35-5	59.07	NH <sub>2</sub>	0.001	Has to our knowledge not been observed as degradation product
Ethylamine	75-04-7	45.08	H <sub>2</sub> N	0.01	Not observed, may form in low concentrations
Dimethylamine	124-40-3	45.08	N H	0.001	Nitrosoform of this compound has been observed, suggesting that this compound has been formed.
Diethylamine	109-89-7	73.14	N H	0.001	Not observed, likelihood of formation comparable to dimethylamine.
1-Butanamine	109-73-9	73.14	NH <sub>2</sub>	0.001	Not observed, likelihood of formation less than for ethylamine.
Dibutylamine	111-92-2	129.24	, , , , , , , , , , , , , , , , , , ,	0.001	Mass consistent with this compound has been observed in pilot-plant liquid samples.
N-methylethanamine	624-78-2	59.11	Hz	0.001	Not observed, likelihood of formation perhaps comparable to ethylamine.
N-methyl 1- butanamine	110-68-9	87.16	N H	0.001	Not observed, likelihood of formation is likely to be low.
N-ethyl 1- butanamine	13360-63- 9	101.19		0.001	Not observed, likelihood of formation is likely to be low.
1-Propanamine	107-10-8	59.11	NH <sub>2</sub>	0.0005	Not observed, likelihood of formation is likely to be low.
Dipropylamine	142-84-7	101.19		0.0001	Not observed, likelihood of formation is likely to be low.
2-methyl-2- (methylamino)- 1- Propanol	27646-80- 6	103.1	HOULUN	0.001	Result of thermal degradation. Expected for TCM solvent 1.

### Table 2.2 Volatile degradation products for MEA and other TCM solvents



In Table 2.3 we list medium volatility degradation product. This list is 22far from complete, for each solvent there may perhaps be 10-50 degradation products that fall in this category. We do however believe the list is representative and we have attempted to include all expected types of degradation products.

This list includes both thermal and oxidative degradation products. Some of these degradation products are transient, reacting to form new degradation products while others accumulate over time.

Since these degradation products are much less volatile than the ones listed in Table 2.2, their emissions are expected to be much lower.

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Degradation product	CAS.	Structure	dG <sub>solv</sub> [kcal/mol]	Type of degradation	Ref./Comment
			[kcal/mol]	product	
Oxazolidine	497-25-6	O NH	-10.1	Result of thermal degradation. Transient degradation product.	Certain degradation product in MEA. Does not appear in large concentration.
1-(2_hydroxyethyl)-2- imidazolidinone (HEIA)	3699-54- 5	HO	-15.0	Result of thermal degradation. Does to some extent accumulate over time.	Certain degradation product in MEA. May be one of the main degradation products.
N-(2- hydroxyethyl)imidazo le (HEI)	1615-14- 1	OH NOH	-14.6	Result of oxidatve degradation. Does to some extent accumulate over time.	Observed in MEA (work of Andrew Sexton and NTNU/SINTEF).
Piperazine	110-85-0	HZ	-7.4	Result of oxidative degradation. Expected to accumulate over time.	Not expected to form to significant degree in MEA. Likely to be significant for 1 TCM solvent. Substituted piperazines may also form.
4,4-dimethyl-2- Oxazolidinone	26654- 39-7	NH O	-5.9	Result of thermal degradation. Transient degradation product.	Expected for 1 TCM solvent.
N-(2-hydroxyethyl)- ethylenediamine, HEED	111-41-1	HO NH <sub>2</sub>	-11.5	Result of thermal degradation. Transient degradation product.	Certain degradation product in MEA. Similar degradation products expected for most TCM solvents.
N-(2-hydroxyethyl)- Formamide (HEF)	693-06-1	H Z O	-11.6	Result of oxidative degradation. Expected to accumulate over time.	Certain degradation product in MEA. Similar degradation products expected in most solvents
N-(2-hydroxyethyl)- acetamide(HEA)	142-26-7	HZ P	-11.1	Result of oxidative degradation. Expected to accumulate over time.	Certain degradation product in MEA. Similar degradation products expected in most solvents
Diethanolamine (DEA)	111-42-2	HO N H	-12.9	Result of thermal degradation.	Expected for 1 TCM solvent.

### Table 2.3. Medium volatility degradation products for MEA and other TCM solvents



In Table 2.4 we have listed non-volatile degradation products. These are mainly organic acids, or molecules having carboxylic acid functionalities. This list is not complete but we believe the listed components are representative.

All these are oxidative degradation products. Most of them are expected to accumulate over time (until solvent reclaiming is carried out).

Degradation product	CAS.	Structure	Ref./Comment
Formic acid	64-18-6	ОН	Certain degradation product in MEA. Expected in most TCM solvents
Acetic acid	64-19-7	ОН	Certain degradation product in MEA. Expected in most TCM solvents
Oxalic acid	144-62-7	но он	Certain degradation product in MEA. Expected in most TCM solvents
N,N-Bis(2- hydroxyethyl)glycine Diethylolglycine/bicine	150-25-4	но он	Expected for 1 TCM solvent. Similar degradation products expected for most solvents.

Table 2.4. Non-volatile degradation products for MEA and other TCM solvents

### 2.1.9 Nitrosamines and nitramines

Table 2.5 shows the detected nitrosamines, and nitrosamines that we expect from our present knowledge of these compounds. The nitrosamines 4-nitroso-morpholine and N-nitrosodiethanolamine were detected in ACCs MEA campaign in Longannet (Rokkjær and Vang 2009). It has also been reported that small quantities (ppb level) of nitrosamines have been detected in a MEA campaign in the Esbjerg plant in Denmark (da Silva and Aas 2009). As shown in Table 2.5, 8 of the 10 nitrosamines are volatile.

From the present state of knowledge it would appear likely that most amine solvents will form some nitrosamines.

Nitrosamine and nitramines are formed as a result of reactions between NOx components and amine species. This means that nitrosamines may form from reaction between NOx in the exhaust gas, the solvent and degradation products. The concentration of NOx in the exhaust gas, the chemical structure of the solvent and the concentration of degradation products are likely to determine the extent of nitrosamine and nitramine formation in a CO<sub>2</sub> capture plant.

The  $CO_2$  absorption process differs significantly from systems where nitrosamines are known to form. The nature of the liquid, pH and temperature in absorption process all differ significantly from that of systems where nitrosamine chemistry has been studied in detail. It is therefore



difficult to draw conclusions on nitrosamine formation under these conditions from data available in the literature. Nitrogen oxide forms a number of species in aqueous solution, the relative concentration of these depend on the pH of the system. This means that the likelihood of nitrosamine formation also may depend on the pH.

We do know that secondary amines may form stable nitrosamines. Tertiary amines may also form stable nitrosamines, but the reactions are expected to be significantly lower than for secondary amines. Primary amines are not expected to form stable nitrosamines. In a solvent system based on primary amines there will however be a certain accumulation of degradation products with secondary and tertiary amine functionality.

This would suggest that overall secondary amines are likely to form the most nitrosamines, while primary amines form the least.

Among the primary amines the risk of nitrosamine formation is probably proportional to the extent of degradation. We could therefore initially assume that for a given NOx content in the exhaust gas the rate of formation of nitrosamines are proportional to the formation rate of ammonia (same assumption as for the volatile compounds). The experimental data on nitrosamine formation in  $CO_2$  capture plants is extremely limited. There are also technical challenges involved in detecting and quantifying the nitrosamines. This is partly due to the fact that these compounds are present in very low concentrations.

For MEA it would seem likely that there are some other nitrosamines formed in addition to those observed so far.

For TCM solvents 4 and 9 we expect higher rates of nitrosamine formation than for MEA.

At present we are not aware that any dedicated work has been done to identify nitramines in degraded amine solvents. Nitramines are also a little studied group of compounds. It is therefore difficult to make any predictions with regards to their formation in a  $CO_2$  capture plant. Based on what we at present know about nitrosamine formation, some degree of nitramine formation would seem likely.

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Degradation product	CAS.	Structure	dG solv <sup>a</sup>	Ref./Comment
			[kcal/mol]	
N-nitrosodimethylamine	62-75-9		-2.6(v)	Likely nitrosamine degradation product. May form in most solvents. Detected in ACCs Longannet campaign
4-nitroso-morpholine	59-89-2	N-N O	-4.4(v)	Detected in ACCs Longannet campaign. May form in most alkanolamine solvents
N-nitrosodiethanolamine	1116-54-7		-9.0(mv)	Detected in ACCs Longannet campaign
n-butyl-n-nitroso-1- Butanamine	924-16-3		0.5(v)	Detected in liquid samples from pilot-plant
N-nitroso-Diethylamine	55-18-5	o <sup>N</sup> N	-0.9(v)	May form in most TCM solvents
N-nitroso N-(2- hydroxyethyl) ethlenediamine	No CAS	H <sub>2</sub> N OH	-9.5(mv)	May form in MEA.
2-(methylnitrosoamino)- Ethanol	26921-68- 6	N OH	-5.5(v)	May form in some TMC solvents
1-Nitrosopiperazine	5632-47-3	HN N N	-7.0(v)	Likely nitrosamine for TCM solvent 4 and 9.
N,N'-dinitrosopiperazine	140-79-4		-5.0(v)	Likely nitrosamine for TCM solvent 4 and 9
N-nitroso N'-aminoethyl piperazine	No CAS		-5.2(v)	Likely nitrosamine for TCM solvent 9

a: v: volatile component, mv: component that is less volatile than MEA

### 2.1.10 Likely Emissions

The emission of a given degradation product depends on concentration of the component, the compounds chemical properties and the design of the capture plant and in particular the water-wash section.

The key properties of the degradation product are:

- Volatility
- Base strength/acid strength
- Affinity to other species present in the liquid

Some degradation products will to varying extents be bound in ionic form in the liquid; an example is acids that are deprotonated at the conditions present in the absorber. These ionic forms



do not have a significant vapor pressure. It is the concentration of the free (uncharged) form of the degradation product and its volatility that will determine its concentration in the gas phase.

The key properties of the capture plant are:

- Design and operation of the water wash
- Extent of entrainment
- Operation of acid wash

The composition of any entrainment emissions is somewhat uncertain. The most conservative assumption is to say that the entrainment has the same composition as that of the liquid phase in the absorber.

The water wash will be most efficient for medium volatility and non volatile degradation products. The water wash will be less efficient for the volatile degradation products.

An acid wash should be efficient in reducing emissions of any compounds that have base strength, like ammonia, alkylamines, solvent components and degradation products with amine functionalities. Experimental data will be required to determine the efficiency of acid-wash units. From what we know today it would seem likely that an acid-wash can reduce emissions of basic components by a factor of 10. Such an acid-wash is not expected to be effective in reducing emissions of nitrosamines and nitramines.

The effect of a acid-wash on nitrosamine emissions is hard to predict and is an issue that should be studied further.

Many medium volatility and non volatile degradation products are likely to be present in concentrations that are less than 1% of the solvent concentration. At the same time many of these components are less volatile than the amine itself by at least an order of magnitude. If for example the solvent emission is at 1 ppm, emissions of such degradation products would be expected to be on 0.0001 ppm level.

The volatility of each component can be estimated with a high degree of confidence with computational chemistry tools. While the concentration of different degradation products in a  $CO_2$  capture plant have in most cases not been quantified, we believe reasonable estimates can be made based on the overall degradation rate (loss of solvent).

For MEA that has a relatively high degradation rate, the main emissions may consist of volatile degradation products. For other TCM solvents that are expected to be less prone to degradation a larger part of the emission may consist of the solvent itself.

### 2.1.11 Recommendations for pilot plant measurements

Further work is required to determine the emissions of nitrosamines and nitramines. Such measurements are demanding and there is the risk of false detection as well as potential issues related to formation or destruction of nitrosamines during sampling.

It would be advantageous to have a group detection method for nitrosamines and nitramines.



In our view sampling should be carried out both of the emissions from the plant and the exhaust gas coming into the plant. This in order to make sure that emissions from the  $CO_2$  capture plant are not confused with emissions from the power plant. Ideally both streams should be sampled for the main components.

LC-MS scan analysis of liquid samples from the water-wash can be used to check if there is any unexpected degradation products being emitted to a significant degree.

#### 2.2 Solvent degradation after emission to air

Degradation after emission to air may appear as the result of photochemical reactions. A theoretical study of the atmospheric degradation of the 4 amines was conducted by NILU (Bråten et al., 2009). This study indicated that a large number of degradation products could be generated, but low amine emissions will result on in small concentrations of degradation products. A number of theoretical photochemical reaction products were identified from the 4 amines included, and several these had a life-time  $\tau_{OH}$  > 3 days in air (see Appendix A). It was also noted that a number of nitrosamines and nitramines could be formed with reactions with NO<sub>2</sub> or NO. Further, components like dimethylamine, which has been identified as a volatile degradation products in the post combustion process (see Table 2.2), has been shown to form nitroso-dimethylamine by reaction with gaseous nitrous acid (Hanst et al., 1977). Several of the compounds were expected to rapidly degrade in daylight. Since most of the nitrosamine and nitramine compounds described in the NILU study were the result of a theoretical study, further actions require evidences from amine emission experiments or from detection through monitoring campaigns.

#### 2.3 Solvent biodegradation products

Amines reaching biotic environments like soil, sediments and water (fresh- or seawater) are subjected to biodegradation through aerobic or anaerobic processes, mainly conducted by the bacteria present in these environments.

A study of several amines in a bioreactor under anoxic conditions showed a number of putative intermediates: Formaldehyde, methanol, formic acid, acetaldehyde, ethanol, acetic acid, glycolaldehyde, glyoxal, glycolicacic acid and glyoxylic acid (Knapp et al., 1996). Studies of MEA in soil or in bioreactors showed successful biodegradation of the amine with ammonium, acetate, ethanol and nitrogen gas as reaction products (Ndegawa et al., 2004; Mrklas et al., 2004). In a recent study the metabolites *N*-(2-anilinoethyl)acetamide and *N*-acetyl-*N*\_-phenylpiperazine were detected during biodegradation of piperazine by a strain of *Mycobacterium* sp. (Adjei et al., 2007).

Predictions of the potential biodegradation products of amines that would be emitted to an oxygen-containing biotic environment may be performed by the Biodegradation/biocatalysis Database of the University of Minnesota (BBD-UM) (http://umbbd.msi.umn.edu/). This database predicts the degradation pathways for organic compounds based on the input of chemical structure or SMILES specification. The essential theoretical degradation products identified by this approach are shown in Appendix B. At least 13 different theoretical reaction products were identified. Some of these were common for several amines, mainly glycolic acid and formaldehyde. In addition ammonium is common, due to its formation during the deamination step. The different products of biodegradation were common organic compounds which entered



well-known microbial metabolisms (e.g. metabolisms for glyoxylate/dicarboxylate, glycerophospholipid, propionate, glycine, serine, threonoine, or pyruvate). In these pathways the products are used for building up biomass, or eventually oxidised to inorganic carbon.

It was noted that some amines relevant for post combustion technology may also be biodegradation products from other amines. Both MEA and piperazine may be the products of other solvent amines.

### **3** Possible environmental and health effects of degradation products

Most of the degradation products described in Tables 2.2-2.5 are common chemicals with HEdata available from several sources. In this report we mainly used the International Uniform ChemicaL Information Database (IUCLID) for data collection. (<u>http://ecb.jrc.ec.europa.eu/esis/index.php?PGM=dat</u>). In cases were IUCLID reports were not available material safety and data sheets (MSDS) were used. However, in some instances neither IUCLID nor MSDS informations were found, and some potential degradation products even missed CAS numbers.

### 3.1 Environmental effects

Ecotoxicity informations for degradation products categorized to volatility are summarised in Table 3.1, 3.2 and 3.3. For some of the products no environmental data were available, or data were limited. In general the products were biodegradable in the range from 30 to 100 % degradability, indicating no or limited persistence in soil or aquatic environments. Only one compound (HEED) showed no degradability. The ecotoxicity data varied considerable, as expected. This reflects different toxicity levels, but also that tests have been performed by different laboratories, by different methods, and with different species within each trophic level (fish and algal species). The ecotoxicity data ranged from 0.02 to 26000 mg/L for fish species, from 25 to 13600 mg/L for *Daphnia*, and from 0.3 to 7000 mg/L for algal species. Variations between tests were higher for volatile than for medium and non-volatile products. The large ranges observed for the volatile compounds may partly be a result of technical difficulties with the exposure of volatile compounds to test organisms.

The combination of expected low emission, water-solubility (low bioaccumulation potentials), biodegradability and low to moderate acute ecotoxicity for most of the post combustion degradation products, should indicate that the environmental risk associated with these products should be moderate or low. However, there is a lack of data for some of the products expected to be persistant (e.g. oxazolidone, HEIA, HEI and bicine), and efforts should be made to investigate the environmental impacts of these products if they are measured in emissions from CO<sub>2</sub> post combustion plants.

Ammonia may be regarded as an inorganic nutrient during microbial metabolism and is expected to be rapidly oxidized to nitrate. Furthermore, ammonia and nitrate may be related to eutrophication processes. Ammonia is a product from the post combustion process (see Table 2.2), but may also form in the environment as the result of biological processes (e.g. deamination of N-containing compounds), as shown in Appendix B. Nitrate may be formed biologically by chemolitotrophic oxidation of ammonia. High input of ammonia to terrestrial, aquatic and marine environments may result in fertilization and unwanted biological changes in the local catchment



area, resulting in changed vegetation, algal blooms, etc. However, such effects will require very high emissions of ammonia in order to compete with other man-made processes like fertilization through agriculture. Environmental data for possible nitrosamines are shown in Table 3.4. Of the nitrosamines described in Table 2.5 data were only found for N-nitrosodimethylamine and N-nitroso-Diethylamine.

	vest are shown in brackets.				
Degradation product	<b>Biodegradability</b>	Ecotoxicity ranges: mg/L EC/LC-50			
Degradation product	(%)	Fish	Daphnia	Algae	
Ammonia	Rapidly degraded to NO <sub>3</sub> (2)	0.024-2.5 (54)	25-189 (3)	13-25 (3)	
Formaldehyde	90 % (1)	27-565 (28)	39-52 (3)	0.3 (1)	
Acetaldehyde	80 % (1)	31-153 (3)	48.3 (1)	236-1270 (6)	
Acetone	84-90 (2)	5540-11000 (3)	7636-12600 (4)	2844-7000 (3)	
Formamide	30-100 % (2)	4600-9135 (2)	> 500 (1)	> 500 (1)	
Methylamine	55-100 % (6)	10-1000 (9)	163-702 (2)	1)	
Acetamide	No data	13000-26000 (1)	1)	1)	
Ethylamine	98-100 % (2)	10-1000 (4)	94-102 (2)	1)	
Dimethylamine	30-100 % (5)	210 (1)	89-105 (1)	9-30 (2)	
Diethylamine	68-75 % (2)	25-1000 (5)	41-164 (4)	20-56 (2)	
1-Butanamine	60-100 % (2)	24-268 (5)	43-75 (2)	1)	
Dibutylamine	94-97 % (1)	5.5-7.6 (2)	66-87 (2)	1.2-19 (3)	
N-methylethanamine	1)	1)	1)	1)	
N-methyl-1-butaneamine	1)	1)	1)	1)	
N-ethyl-1-butanamine	1)	1)	1)	1)	
1-Propanamine	"Biodegradable"	46 (1)	70.7 (1)	1)	
Dipropylamine	30-100 % (3)	20-60 (1)	73-77 (2)	5.4 (1)	

# Table 3.1Environmental data for volatile degradation products<br/>based on data from IUCLID, ECOTOX or HE-sheets. The numbers of test<br/>results from each ecotoxicity test are shown in brackets.

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Table 3.2	Environmental data for medium volatile degradation products
	based on data from IUCLID, ECOTOX or HE-sheets. The numbers of test
	results from each ecotoxicity test are shown in brackets.

	Biodegradability	Ecotoxicity ranges: mg/L EC/LC-50 (no tests)				
Degradation product	(%)	Fish	Daphnia	Algae		
Oxazolidine	1)	1)	1)	1)		
1-(2-hydroxyethyl)-2- imidazolidinone (HEIA)	1)	1)	1)	1)		
N-(2-hydroxyethyl) imidazole (HEI)	1)	1)	1)	1)		
Piperazine	90 % (1)	52-159 (1)	1)	472 (1)		
4,4-dimethyl-2- oxazolidinone	1)	1)	1)	1)		
N-(2-hydroxyethyl)- ethylenediamine, HEED	0 % (1)	728 (1)	22-225 (3)	210 (1)		
2-methyl-2- (methyloamino)-1- propanol	1)	1)	1)	1)		
N-(2-hydroxyethyl)- formamide (HEF)	1)	1)	1)	1)		
N-(2-hydroxyethyl)- acetamide (HEA)	1)	1)	1)	1)		
Diethanolamine (DEA)	93-97 (3)	800-1850 (6)	1.4-289 (9)	2.1-548 (5)		

<sup>1)</sup>No data in IUCLID or HE-sheets

# Table 3.3Environmental data for non-volatile degradation products<br/>based on data from IUCLID, ECOTOX or HE-sheets. The numbers of test<br/>results from each ecotoxicity test are shown in brackets.

	Biodegradability	Ecotoxicity ranges: mg/L EC/LC-50 (no tests)				
Degradation product	(%)	Fish	Daphnia	Algae		
Formic acid	98-100	122	120-151	25-27		
	(2)	(1)	(2)	(2)		
Acetic acid	95 %	50-500	32-6400	73-4000		
	(2)	(5)	(5)	(7)		
Oxalic acid	40 %	160	137	80		
	(1)	(1)	(1)	(1)		
N,N-Bis(2- hydroxyethyl)glycine Diethylolglycine/bicine	1)	1)	1)	1)		

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Environmental data for possible nitrosamine degradation products, based on Table 3.4 data from IUCLID, ECOTOX, SRC Environmental Fate Database or HEsheets. The numbers of test results from each ecotoxicity test are shown in brackets.

Drackets.						
	Biodegradability	Ecotoxicity ranges: mg/L EC/LC-50 (no tests)				
Degradation product	(%)	Fish	Daphnia	Algae		
N-nitrosodimethylamine	Judged as biodegradable	832-1062	280-445 <sup>2)</sup> (4)	4.0-51 (2)		
4-nitroso-morpholine	1)	75-100 <sup>3)</sup>	1)	1)		
N-nitrosodiethanolamine <sup>4)</sup>	1)	1)	1)	1)		
n-butyl-n-nitroso-1- Butanamine	1)	1)	1)	800 <sup>5)</sup> (1)		
N-nitroso-Diethylamine	Judged as biodegradable	775	500 <sup>2)</sup> (1)	10.2		
N-nitroso N-(2- hydroxyethyl) ethlenediamine	1)	1)	1)	1)		
2-(methylnitrosoamino)- Ethanol	1)	1)	1)	1)		
1-Nitrosopiperazine	1)	1)	1)	1)		
N,N'-dinitrosopiperazine	1)	1)	1)	170 (1)		
N-nitroso N'-aminoethyl piperazine	1)	1)	1)	1)		

<sup>1)</sup> No data in IUCLID or HE-sheets
<sup>2)</sup> Results from tests with the copepod Gammarus
<sup>3)</sup> Tumor development
<sup>4)</sup> Amphibian genotoxicity: 6.2-12.6 mg/L

<sup>5)</sup>Genotoxicity NOEC

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### 3.2 Health-related data

Health-related data were also collected from IUCLID and HSE-sheets for the degradation products and results shown in Tables 3.9 to 3.11 for the three volatility categories.

The data for acute oral or dermal toxicities varied from 7 to > 10000 mg/kg bw, with the highest acute toxicity reported for acetamide. Most of the degradation products showed LD50 values lower than 2000 mg/kg bw.

Also other products than the nitrosamines were mutagenic. Both volatile aldehydes (formaldehyde, acetaldehyde) and alkylamines (methylamine, ethylamine, dimethylamine and dibutylamine) showed positive or ambiguous results in these tests. Several of the tests for mutagenicity showed ambiguous results, indicating that it was difficult to predict whether the test results were positive or negative. If this was caused by test procedures which are difficult to predict, or by the quality of performance, is impossible for us to know.

Only a few data results of reproduction toxicity were found for the degradation products. Noobserved adverse effect limits (NOAEL-values) are given for reproduction toxicity and repeated dose toxicity. These NOAEL-values varied from 350 to > 5000 mg/kg bw, formamide showing the lowest value. Some of the results were shown as mg/l (e.g. for DEA), and will not be comparable to the other results.

Also for repeated dose toxicity NOAEL values were presented as mg/kg bw or as mg/L. The mg/L-results varied from 0.006 to 6200 mg//L, but exposure regimes and exposure periods were different between tests, and several of the results are therefore difficult to compare. The products with the lowest NOAEL concentrations were formaldehyde, several amide/amines (formamide, methylamine, ethylamine, dimethylamine) and the formic acid. For products with NOAEL of mg/kg bw units, two degradation products showed NOAEL lower than 1000 mg/kg bw (piperazine and acetic acid).

Most of the degradation products were corrosive and/or irritating to skin and eye, while only some of these showed sensitisation characteristics.

The health-related data for potential nitrosamines are shown in Table 3.12. Only a few data were available from common databases or from MSDS. Data for mutagenicity and gentoxicity were found in the database GENE-TOX for several of these compounds, showing positive results for all of them. Nitroamines and nitramines as possible amine degradation products have received attention due to their potential carcinogenic effects. During a recent literature study HE information of the theoretical nitrosamines products were described (Bråten et al., 2007, Låg et al., 2009).

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Degradation product	Acute toxicity-LD50 (ED50; mg/kg bw)	Mutagenicity/ Genotoxicity	Reproduction toxicity	Irritation/ Corrosion	Sensitization	Repeated dose toxicity (NOAEL)
Ammonia	Oral: 350 Dermal: No data	Negative	1)	Eye irritant	Negative	300- 1247 mg/L
Formaldehyde	Oral: 100->7000 Dermal: 2-270	Positive	Negative	Skin: positive Eye: positive	Ambiguous	0.006-0.077 mg/L
Acetaldehyde	Oral: 1939 Dermal: No data	Ames test: Pos/Neg Mamm. Cytogen: Positive	Negative to ambiguous	Skin: Negative Eye: Positive	Positive	125-150 mg/L
Acetone	Oral: 1800-9800 Dermal: > 10000	Ames test: Negative Mamm. Cytogen: Neg/Pos	NOAEL teratogen: 2200 mg/L	Skin: Positive Eye. Positive	Negative	100-2500 mg/L
Formamide	Oral: 3200-7932 Dermal: > 10000	Ames test: Negative Mamm. Cytogen: Neg/Ambig	NOAEL 750 mg/L parenal/350 mg/L offspring	Skin: Pos/neg Eye. Positive	Negative	0.19-113 mg/L
Methylamine	Oral: 80-698 Dermal: No data	Ames test: Negative Mamm. Cytogen: Positive	NOAEL> 5 mg/kg bw	Skin: Positive Eye. Positive	1)	0.096 mg/L
Acetamide	Oral: 7 mg/kg Dermal: No data	Ames test: Negative Mamm. Cytogen: Positive	1)	1)	1)	1)
Ethylamine	Oral: 400->3200 Dermal: 265-360	Ames test: Neg- ambiguous Mamm. Cytogen: Positive	1)	Skin: Positiv Eye: Positive	1)	0.18 mg/L
Dimethylamine	Oral: 698-8100 Dermal: 3900	Ames test: Neg/pos Mamm. Cytogen: Neg/ambig	NOAEL maternal and teratogenic >225 mg/kg bw	Skin: Positive Eye. Positive	Positive	0.02-0.19 mg/L
Diethylamine	Oral: 540-1000 Dermal: 12.1-17.3	Ames test: Negative Mammalian: No data	1)	Skin: Positive Eye: Positive	Negative	0.076 mg/L
1-Butanamine	Oral: 366-720 Dermal: 850	Amest test: Negative Mammalian: Negative	1)	Skin: Positive Eye: Positive	Negative	1)

### Table 3.5Health-related data for volatile degradation products (see Table 3.1) based on IUCLID or HE-sheets



### Table 3.5Continued

Degradation product	Acute toxicity-LD50 (ED50; mg/kg bw)	Mutagenicity/ Genotoxicity	Reproduction toxicity	Irritation/ Corrosion	Sensitization	Repeated dose toxicity (NOAEL)
Dibutylamine	Oral: 189-550 Dermal: 768-1010	Ames test: Negative Mamm. Cytogen: Pos/ambig	1)	Skin: Positive Eye: Positive	Negative	1)
N-methylethanamine	No data	1)	1)	1)	1)	1)
N-methyl-1-butaneamine	Oral: 420 Dermal: 627	1)	1)	Skin: Positive Eye: Positive	1)	1)
N-ethyl-1-butanamine	Oral: 310 Dermal: No data	1)	1)	No data	1)	1)
1-Propanamine	Oral: 370 Dermal: 410	1)	1)	Skin: Positive Eye: Positive	1)	1)
Dipropylamine	Oral: 200-1600 Dermal: 925	Ames test: Negative Mamm. Cytogen: Negative	1)	Skin: Positive Eye: Positive	Negative	1)

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Table 3.6	Health-related data for medium volatile degradation products (see Table 3.2) based on IUCLID or HE-sheets
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Degradation product	Acute toxicity-LD50 (ED50; mg/kg bw)	Mutagenicity/ Genotoxicity	Reproduction toxicity	Irritation/ Corrosion	Sensitization	Repeated dose toxicity (NOAEL)
Oxazolidine	1)	Carcinogenicity: Equivocal	1)	1)	1)	1)
1-(2_hydroxyethyl)-2- imidazolidinone (HEIA)	1)	1)	1)	1)	1)	1)
N-(2- hydroxyethyl)imidazole (HEI)	1)	1)	1)	1)	1)	1)
Piperazine	Oral: 2500-4500 Dermal: 4000	Ames test: Neg/pos Mamm. Cytogen: Negative	NOAEL maternal and teratogenic: >5000 mg/kg bw	Skin: Positive Eye. Positive	Positive	75 mg/kg bw
4,4-dimethyl-2- oxazolidinone	1)	1)	1)	1)	1)	1)
N-(2-hydroxyethyl)- ethylenediamine, HEED	Oral: 2150-3014 Dermal: 2000	Ames test: Neg/pos Mamm. Cytogen: Negative	Developmental: cardiovascular	Skin: Positive Eye. Positive	Positive	1000 mg/kg bw
2-methyl-2- (methyloamino)-1- propanol	1)	1)	1)	1)	1)	1)
N-(2-hydroxyethyl)- formamide (HEF)	1)	1)	1)	1)	1)	1)
N-(2-hydroxyethyl)- acetamidee (HEA)	Oral: 26950 Dermal: 500	1)	1)	1)	Skin: Mild Eye: Severe	1)
Diethanolamine (DEA)	Oral: 780-3460 Dermal: 12200-13000	Ames test: Negative Mamm. Cytogen: Negative	NOAEL 0.05 mg/L maternal and teratogenic	Skin: Negative Eye. Positive	Negative	< 32 mg/kg bw

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Table 3.7Health-related data for medium non-volatile degradation products (see Table 3.3) based on IUCLID or HE-sheets

Degradation product	Acute toxicity-LD50 (ED50; mg/kg bw)	Mutagenicity/ Genotoxicity	Reproduction toxicity	Irritation/ Corrosion	Sensitization	Repeated dose toxicity (NOAEL)
Formic acid	Oral: 730 Dermal: No data	Ames test: Negative Mamm. Cytogen: Neg-ambiguous	NOAEL > 128 mg/L	Skin: Positive Eye. Positive	1)	0.06 mg/L
Acetic acid	Oral: 3310-3530 Dermal: 1060	Ames test: Negative Mamm. Cytogen: Negative	NOAEL > 1600 mg/kg bw	Skin: Positive Eye. Positive	1)	210 mg/kg bw
Oxalic acid	Oral: 375-7500 Dermal: 20000	Ames test: Negative Mamm. Cytogen: No data	NOAEL > 8400 mg/kg bw	Skin: Positive Eye. Positive	1)	< 500 mg daily oral intake
N,N-Bis(2- hydroxyethyl)glycine Diethylolglycine/bicine	Intraperitonal: 1540 mg/kg bw	1)	1)	1)	1)	1)



Table 3.8	Health related data for possible nitrosamine degradation products based on ecotoxicity results (Tables 3.4) and species used for
	calculations. Results for mutagenicity/genotoxicity were collected from the Gene-Tox database of US EPA.

Degradation product	Acute toxicity-LD50 (ED50; mg/kg bw)	Mutagenicity/ Genotoxicity	Reproduction toxicity	Irritation/ corrosion	Sensitization	Repeated dose toxicity (NOAEL)
N-nitrosodimethylamine	Oral: 37.0 Dermal: 15.0	Ames test: Positive Mamm. Cytogen: Postive Carcinogenic	Fetotoxic	1)	1)	1)
4-nitroso-morpholine	Oral: 282 Dermal: 170	Ames test: Positive Mamm. Cytogen: Postive Carcinogenic	1)	1)	1)	1)
N-nitrosodiethanolamine	Oral: 7500 Dermal: 11000 (hamster)	Ames test: No data Mamm. Cytogen: Postive/ambigous	Expected toxic	1)	1)	1)
n-butyl-n-nitroso-1- Butanamine	Oral: 1200 Dermal: 1200	Ames test: No data Mamm. Cytogen: Postive/ambigous Carcinogenic	Fetotoxic	1)	1)	1)
N-nitroso-Diethylamine	Oral: 220 Dermal: 195	Ames test: Positive Mamm. Cytogen: Postive Carcinogenic	Fetotoxic	Skin: Positive Eye. Positive		
N-nitroso N-(2- hydroxyethyl) ethlenediamine	1)	1)	1)	1)	1)	1)
2-(methylnitrosoamino)- Ethanol	1)	Mutagenic Carcinogenic	Expected toxic	1)	1)	1)
1-Nitrosopiperazine	Oral: 2260 Dermal: No data	Ames test: Positive Mamm. Cytogen: No data Carcinogenic	1)	1)	1)	1)
N,N'-dinitrosopiperazine	1)	1)	1)	1)	1)	1)
N-nitroso N'-aminoethyl piperazine	1)	1)	1)	1)	1)	1)

#### **3.3 PNECs and DNELs of degradation products**

The hazard of a chemical can be determined as the "*predicted no-effect concentration*" (PNEC) or the "*derived no-effect level*"(DNEL) for ecotoxicity and health toxicity, respectively, as envisaged in Appendix I of the REACH Directive EC 1907/2006 and the Technical Guidance documents (TGD, 2003). For both hazard systems available toxicity data are used and divided by safety assessment factors. For PNEC determinations an assessment factor of 1000 is mainly used (exceptions are noted for individual compoynds) with data from at least one short-term ecotoxicity test from each of three trophic levels. DNEL calculations are not as straightforward, since an overall assessment factor is calculated from a number of individual assessment factors, depending on the exposure conditions. However, until agreement on calculations a tier I assessment factor of 1200 is used here. This assessment factor has been suggested to be used as a simple "non-expert" way of generating as a first screening DNEL, using a derived simple assessment factor large enough to cover all populations and long-term exposure (CSA Coping studies; <u>www.wvmetalle.de/wvmprofi/docs/ doc 4550\_2007621121829.pdf</u>). Typical dose descriptors for DNEL calculations are NOAEL of reproduction toxicity, which we also have used here for DNEL calculations.

The results of PNEC and DNEL calculations are shown in Table 3.9-3.12.

The PNEC calculations showed that the most sensitive organisms for individual degradation products were found within all three trophical levels (algae, invertebrates and fish), and varied from 0.000024 to 13 mg/L. The degradation products with the lowest PNEC-values (< 0.01 mg/L) were ammonia, formaldehyde, dimethylamine and DEA. All these, except DEA, are volatile degradation products. These products are expected to biodegrade after emission (biodegradation data ranging from 30 to 100 %).

Few reproduction toxicity data were available for DNEL calculations, and the degradation products with the lowest DNEL concentrations were methylamine and dimethylamine. This was partly caused by low upper concentrations used in the test for these products.

# Table 3.9PNEC and DNEL calculations of volatile degradation products based on<br/>ecotoxicity results (Tables 3.1) and reproduction toxicity (Table 3.5). For<br/>DNEL data not related to animal bodyweight (bw) were excluded.

	PNEC		DNEL
Degradation product	Conc. (mg/L)	Species	Conc (mg/kg bw)
Ammonia	0.000024	Lepomis macrochirus (freshwater fish)	1)
Formaldehyde	0.0003	Scenedesmus sp. (freshwater algae)	1)
Acetaldehyde	0.0308	Pimephales promelas (freshwater fish)	1)
Acetone	2.84	Anabena cylindica (algae)	1)
Formamide	4.6	Leuciscus idus (freshwater fish)	1)
Methylamine	0.010	Semolitus astromaculatus (freshwater fish)	0.0042
Acetamide	13	Mosquito fish (freshwater fish)	1)
Ethylamine	0.010	Pimephales promalas (freshwater fish)	1)
Dimethylamine	0.009	Selenastrum capricornutum (algae)	0.19
Diethylamine	0.020	Selenastrum capricornutum (algae)	1)
1-Butanamine	0.024	Menidia berrylina (freshwater fish)	1)
Dibutylamine	0.0012	Scenedesmus subspicatum (phytoplankton)	1)
N-methylethanamine	1)		1)
N-methyl-1-butaneamine	1)		1)
N-ethyl-1-butanamine	1)		1)
1-Propanamine	0.046	Leuciscus idus (freshwater fish)	1)
Dipropylamine	0.0054	Scenedesmus subspicatum (phytoplankton)	1)

<sup>1)</sup> No data in IUCLID or HE-sheets

## Table 3.10PNEC and DNEL calculations of medium volatile degradation products based<br/>on ecotoxicity results (Tables 3.2) and reproduction toxicity (Table 3.6). For<br/>DNEL data not related to animal bodyweight (bw) were excluded.

	PNEC		DNEL
Degradation product	Conc. (mg/L)	Species	Conc. (mg/kg bw)
Oxazolidine	1)		1)
1-(2_hydroxyethyl)-2- imidazolidinone (HEIA)	1)		1)
N-(2- hydroxyethyl)imidazole (HEI)	1)		1)
Piperazine	0.052	Cyprinus carpio (freshwater fish)	4.17
4,4-dimethyl-2- oxazolidinone	1)		1)
N-(2-hydroxyethyl)- ethylenediamine, HEED	0.210	Daphnia magna (freshwater invertebrate)	1)
2-methyl-2- (methyloamino)-1- propanol	1)		1)
N-(2-hydroxyethyl)- formamide (HEF)	1)		1)
N-(2-hydroxyethyl)- acetamide (HEA)	1)		1)
Diethanolamine (DEA)	0.0014	Daphnia magna (freshwater invertebrate)	1)

<sup>1)</sup> No data in IUCLID or HE-sheets

Table 3.11PNEC and DNEL calculations of nonvolatile degradation products based on<br/>ecotoxicity results (Tables 3.3) and reproduction toxicity (Table 3.7). For<br/>DNEL only data related to animal bodyweigh (bw) have been used. For DNEL<br/>data not related to animal bodyweight (bw) were excluded.

		PNEC	DNEL
Degradation product	Conc. (mg/L)	Species	Conc. (mg/kg bw)
Formic acid	0.025	Scenedesmus subspicatus (freshwater algae)	1)
Acetic acid	0.032	Artemia salina (marine invertebrate)	1.33
Oxalic acid	0.137	Daphnia magna (freshwater invertebrate)	7.0
N,N-bis/2- hydroxyethyl)glycine Diethylglycine/bicine	1)		1)

<sup>1)</sup> No data in IUCLID or HE-sheets

<b>Table 3.12</b>	PNEC and DNEL calculations of possible nitrosamines based on ecotoxicity
	results (Tables 3.4) and reproduction toxicity (Table 3.8).

		PNEC	DNEL	
Degradation product	Conc. (mg/L)	Species	Conc. (mg/kg bw)	
N-nitrosodimethylamine	0.004	Pseudokirchnerella subcapitata	1)	
4-nitroso-morpholine	<b>0.075</b> <sup>2)</sup>	Danio rerio (freshwater fish)	1)	
N-nitrosodiethanolamine	1)		1)	
n-butyl-n-nitroso-1- Butanamine	1)		1)	
N-nitroso-Diethylamine	0.010	Pseudokirchnerella subcapitata	1)	
N-nitroso N-(2- hydroxyethyl) ethlenediamine	1)		1)	
2-(methylnitrosoamino)- Ethanol	1)		1)	
1-Nitrosopiperazine	1)		1)	
N,N'-dinitrosopiperazine	0.17	Poecilia reticulata (freshwater fish)	1)	
N-nitroso N'-aminoethyl piperazine	1)		1)	

<sup>1)</sup> No data in IUCLID or HE-sheets
 <sup>2)</sup> Long-term effect (tumor development); assessment factor of 100 used

#### 4 Degradation products from selected solvents

#### 4.1 Identification of products

A number 5 of solvents relevant for TCM were selected for closer health-related examination. These solvents are described in a separate report (Brakstad et al., 2010). These solvents may generate a variety of degradation products, and expected amine degradation products from each of these solvents are shown in Table 4.1 to 4.5. A compiled list is shown in Appendix C.

### Table 4.1Expected amine degradation products from MEA. The products are separated<br/>in nitrosamines (blue), nitramines (pink) and amines/amides (green).

Degradation product	CAS.	Structure	<sup>A)</sup> dG solv
N-nitrosodimethylamine	62-75-9		-2.6(v)
4-nitroso-morpholine	59-89-2		-4.4(v)
N-nitrosodiethanolamine	1116-54-7		-9.0(mv)
2-(methylnitrosoamino)- Ethanol	26921-68-6	N N OH	-5.5(v)
Dimethylnitramine	4164-28-7		-3.7
Methylamine	74-89-5	H <sub>2</sub> N——	V
Dimethylamine	124-40-3	ZI	V
Ethylamine	75-04-7	H <sub>2</sub> N	v

Table 4.1 Expect		uation products from MI	(
Degradation product	CAS.	Structure	<sup>A)</sup> dG solv
Diethanolamine (DEA)	111-42-2	HO NH OH	-12.9
N-(2-hydroxyethyl)- Formamide (HEF)	693-06-1	HO	-11.6
N-(2- hydroxyethyl)imidazole (HEI)	1615-14-1	Л Л ОН	-14.6
2-methylaminoethanol	109-83-1	Н ОН	

#### Table 4.1 Expected amine degradation products from MEA (continued).

### Table 4.2Expected amine degradation products from S1. The products are separated<br/>in nitrosamines (blue), nitramines (pink) and amines/amides (green).

Degradation product	CAS.	Structure	<sup>A)</sup> dG solv
N-nitrosodimethylamine	62-75-9		-2.6(v)
Dimethylnitramine	4164-28-7	° z-z	-3.7
Methylamine	74-89-5	H <sub>2</sub> N——	V
Dimethylamine	124-40-3	Z I	V
2-methyl-2- (methylamino)- 1- Propanol	27646-80-6	H Z H	
Ethylamine	75-04-7	H <sub>2</sub> N	V
4,4-dimethyl-2- Oxazolidinone	26654-39-7	NH O	-5.9

Table 4.3	Expected amine degradation products from S3. The products are separated
	in nitrosamines (blue), nitramines (pink) and amines/amides (green).

Degradation product	CAS.	Structure	<sup>A)</sup> dG solv
N-nitrosodimethylamine	62-75-9	N N N N N N N N N N N N N N N N N N N	-2.6(v)
4-nitroso-morpholine	59-89-2		-4.4(v)
N-nitrosodiethanolamine	1116-54-7	от и поредели и поре	- 9.0(mv)
2-(methylnitrosoamino)- Ethanol	26921-68-6	N N OH	-5.5(v)
Dimethylnitramine	4164-28-7	, z – z	-3.7
Methylamine	74-89-5	H <sub>2</sub> N	V
Dimethylamine	124-40-3	N H	V
Ethylamine	75-04-7	H <sub>2</sub> N	V
4-methyl-1- Piperazineethanol	5464-12-0	HO	

Table 4.5 Expect	ca annie acgra	dation products from S5	(continueu).
Degradation product	CAS.	Structure	dG solv
Diethanolamine (DEA)	111-42-2	Но ОН	-12.9
N-(2-hydroxyethyl)- Formamide (HEF)	693-06-1	HO	-11.6
N-(2- hydroxyethyl)imidazole (HEI)	1615-14-1	ОН	-14.6
Hydroxyethyl oxazolidone (HEO)	3356-88-5	HONNO	
1-hydroxyethyl-3- methyl imidazolidone	22455-69-2	HO	
2-methylaminoethanol	109-83-1	Н ОН	
1,2-Ethanediol or ethyleneglycol (EG)	107-21-1	но	
N,N- dimethylethanolamine	108-01-0	HONN	
2,2'-[[2-[(2- hydroxyethyl)methylami no]ethyl]imino]bis- Ethanol (MTHEED)	187731-33-5	но и он	

#### Table 4.3Expected amine degradation products from S3 (continued).

Table 4.4	Expected amine degradation products from S4. The products are separated
	in nitrosamines (blue), nitramines (pink) and amines/amides (green).

in nitrosamines (blue), nitramines (pink) and amines/amides (green).								
Degradation product	CAS.	Structure	<sup>A)</sup> dG solv					
N-nitrosodimethylamine	62-75-9		-2.6(v)					
1-Nitrosopiperazine	5632-47-3	HN N N	-7.0(v)					
N,N'-dinitrosopiperazine	140-79-4		-5.0(v)					
1-nitro-piperazine	42499-41-2		-8.0					
N,N'-Dinitropiperazine	4164-37-8		-3.9					
Dimethylnitramine	4164-28-7		-3.7					
Methylamine	74-89-5	H <sub>2</sub> N——	V					
Dimethylamine	124-40-3	zτ	V					
Ethylamine	75-04-7	H <sub>2</sub> N	V					
Piperazine	110-85-0	HNNH	-7.4					
1,2 Ethylenediamine	107-15-3	H <sub>2</sub> N NH <sub>2</sub>						

Table 4.5	Expected amine degradation products from S9. The products are separated
	in nitrosamines (blue), nitramines (pink) and amines/amides (green).

Degradation product	CAS.	Structure	<sup>A)</sup> dG solv
N-nitrosodimethylamine	62-75-9	N O	-2.6(v)
1-Nitrosopiperazine	5632-47-3	HN N N	-7.0(v)
N,N'-dinitrosopiperazine	140-79-4		-5.0(v)
N-nitroso N'-aminoethyl piperazine	No CAS		-5.2(v)
1-nitro-piperazine	42499-41-2	HN N N	-8.0
N,N'-Dinitropiperazine	4164-37-8	N-N N-N	-3.9
Dimethylnitramine	4164-28-7		-3.7
Methylamine	74-89-5	H <sub>2</sub> N	v
Dimethylamine	124-40-3	Z T	v
Ethylamine	75-04-7	2H2N	V
Piperazine	110-85-0	HNNH	-7.4
1,2 Ethylenediamine	107-15-3	H <sub>2</sub> N NH <sub>2</sub>	

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#### 4.2 Mammalian toxicology – human health hazard

#### 4.2.1 Explanation for classification of long term health hazards

Explanation for classification of long term health hazards is adopted form GESAMP-EHS: : <u>http://www.gesamp.org/publications/publicationdisplaypages/rs64</u>

#### Carcinogenic

The term carcinogenic denotes substances or mixtures that are presumed to induce cancer or to increase its incidence in humans. Evidence to substantiate the notation "carcinogenic" should be available from epidemiological studies and/or from well conducted studies in experimental animals. On a case by case basis, scientific judgment may warrant a decision of presumed human carcinogenicity (C) derived from studies showing limited evidence in humans with limited evidence in experimental animals.

#### Mutagenic

A mutation is a permanent change in the amount or structure of the genetic material in a cell. The term mutation applies to genetic changes both for somatic cells and for germ cells that may give rise to subsequent adverse changes at the phenotypic level. The term mutagenic denotes substances or mixtures that can give rise to an increased occurrence of mutations *in vivo*, in populations of cells and/or organisms. Evidence to substantiate a notation of "mutagenicity" (M) is normally provided from studies conducted *in vivo* on mammalian somatic cells or germ cells. It is recognized that genetic events are central in the overall process of cancer development. Therefore, evidence of mutagenicity indicates that a substance has a potential to induce carcinogenic effects.

#### Reprotoxic

Reproductive toxicity includes adverse effects on sexual function and fertility in adult males and females or on the development of the offspring. The notation "reprotoxic" (R) includes substances for which there is reliable evidence from human experience or from experimental animals of an adverse effect on reproductive ability, capacity, or on development of the offspring in the absence of other toxic effects.

#### Sensitiser

The term sensitising denotes substances or mixtures, which can induce a condition of hypersensitivity in individuals following inhalation (respiratory sensitiser) or skin contact (contact sensitiser). Evidence to substantiate a notation of "sensitising" (S) should be available from human experience and/or from appropriate studies using experimental animals. The term photosensitising (Sp) denotes substances or mixtures that require light to become active and may subsequently induce a condition of contact sensitivity. Evidence to substantiate the notation of "photosensitizing" should be available from human experience and/or from appropriate studies using experimental animals.

#### 4.2.2 Explanation of summary results

The summary table (Table 4.7) condenses the results from the databases which have been examined. The table A complete health hazard report is given in Appendix D, while complete lists of health hazards for individual degradation products are shown in Appendix E. Complete data set are given in Appendix F. For classification and numerical rating the definitions used by



GESAMP/EHS have been used. GESAMP is an organization for cooperation between several UN organizations (UNEP, FAO, UNESCO, IOC, WHO, WMO, IMO, IAEA). GESAMP/EHS was established in 1974 and have carried out detailed examination on roughly 3000 compounds and products carried at sea. The GESAMP classification is carried out by a team of international experts on chemistry, marine ecotoxicity and human health hazard assessment. The experts are invited by IMO (International Maritime Organization) on behalf of GESAMP. Their classification has been published as the GESAMP Composite list by IMO. The GESAMP/EHS review is based on public records as well as confidential company information. In some cases laboratory reports from the toxicity studies have been examined. The files supporting the decisions of the GESAMP/EHS group is located at IMO, London, UK.

Although the GESAMP/EHS profile is generated in order to regulate the safe transport of chemicals at sea, the information on human can be used also for other purposes.

#### 4.2.2.1 Principles of evaluation

In the present project exposure to humans may occur in an occupational setting or as a result of chemicals being dispersed to the neighborhood of the production plant. Any controversy as to exposure limits etc will most probably be focused on the neighborhood environment. Thus, acute oral and dermal toxicity will play a minor role in the final overall assessment. Acute (4 hours) inhalation data will of course be important in any setting where atmospheric exposure is the prime source. However, acute short term exposure at relatively high concentrations may not be a good indicator of health hazards which may occur after low level and long term exposure.

At low level and long term exposure the following health hazards will be of prime interest when regulations are set for permissible exposure to population at or near a plant:

- Carcinogenicity (C)
- Mutagenicity (M)
- Reproductive effects (R)
- Sensitization, primarily by inhalation (S)

The overall assessment of these substances has been suggested in the "comments" and "prio" columns. The two columns taken together should offer some advice to the future development of risk analysis scenarios as well as limits for acceptable atmospheric release and resulting environmental exposure to humans.

The "Prio" column summarizes two indicators – a letter and a number. The letter is an abbreviated assessment of the data which have been found in the available databases:

А	Inadequate data for assessment of hazard
В	Inadequate data for assessment of hazard. Further data may be found in e.g.
	company records
C	Adequate data for hazard evaluation

The number is a provisional estimation of long term health risk relative to air contamination. The numerical value reflects data regarding important long term health issues:

С	Shown to induce or increase cancer in animals or man
М	Shown to cause increased incidence of permanent changes in the amount or



	structure of the genetic material
R	Shown to cause adverse effects on reproductive ability or capacity, or the
	development of offspring
S	Shown to be a sensitizer (skin or respiratory)

A summary evaluation of these risks is then given a numerical value:

0	None or very low long term health risk
1	Low long term health risk
2	Medium long term health risk
3	High long term health risk
4	Very high long term health risk

 Table 4.6
 Databases and explanation of health hazard terms used in Table 4.7

Column heading	Explanation					
Data bases	A "+" indicates that information was found. A "-" indicates that a search was done without finding any relevant information.					
	RTECS: <u>http://ccinfoweb.ccohs.ca/rtecs/search.html</u>					
	IUCLID data sheet: <u>http://ecb.jrc.ec.europa.eu/esis/</u>					
	GESAMP-list: http://www.imo.org/includes/blastDataOnly.asp/data_id%3D25672/Report-BLGCirc.29annex6doc.pdf					
	GESAMP background info: http://www.gesamp.org/publications/publicationdisplaypages/rs64					
	CPDB: <u>http://potency.berkeley.edu/chemicalsummary.html</u>					
	Toxnet: http://toxnet.nlm.nih.gov/index.html checked for all compounds without data. No further data found.					
	EPA-IRIS: http://www.epa.gov/ncea/iris/index.html					
Oral	<b>Oral toxicity LD50 rating codes</b> 0: >2000 1: 300-2000 2: 50-300 3: 5-50 4: <5 mg/kg bw					
Dermal	Percutaneous toxicity LD50 rating codes 0: >2000 1: 1000-2000 2: 200-1000 3. 50-200 4: <50 mg/kg bw					
Inhal	Inhalation toxicity LC50 4 hours exposure rating codes 0: >20 1: 10-20 2: 2-10 3: 0.5-2 4: <0.5 mg/l (4hrs)					
Long term	Full description of rationale for rating given at bottom of table. Short form rating code:					
	C: Shown to induce or increase cancer in animals or man					
	M: Shown to cause increased incidence of permanent changes in the amount or structure of the genetic material					
	R: Shown to cause adverse effects on reproductive ability or capacity, or the development of offspring					
	S: Shown to be a sensitizer					
Comments	A summary expert opinion on the chemical is given in the comments column. For oral/dermal/inhalation the numbers in respective columns indicate:					
	• Negligible toxicity: 0					
	• Slight toxicity: 1					
	Moderate toxicity: 2					
	• Moderately high toxicity: 3					
	• High toxicity: 4					
	Ratings in brackets: Provisional ratings based on limited or no data. Expert judgment.					
	OEL: Occupational exposure level – TWA will be used if available. TWA: time weight average (of exposure for 8 hours)					
	Conclusions and recommendations written in italic bold					
Prio	Expert opinion based on data for the compound it self and chemically similar structures.					
	Abbreviated assessment of data available:					
	A: Inadequate data for assessment of hazard					
	B: Inadequate data for assessment of hazard. Further data may be found					
	C: Adequate data for hazard evaluation					
	Provisional estimation of potential long term health risk relative to ambient air contamination from plant operation:					
	0: None 1: Low 2: Medium 3: High 4: Very high					



Table 4.7Condensed table showing health hazard of some degradation products identified in the CO2-capture process - Mammalian toxicology.<br/>The products are separated in nitrosamines (blue), nitramines (pink), amines/amides (green), and other compounds (brown). For details<br/>of each degradation products – see Appendix F. For each compound group a hazard profile is suggested for a "not otherwise specified"<br/>(NOS) compound representing the group.

Degradation product	CAS.	Structure	Possible solvent origin	Data bases	Oral	Dermal	Inhal	Long term	Comment on human health hazard	Prio
N-nitrosodimethyl- amine	62-75-9		MEA S1 S3 S4 S9 Detected in ACCs Longannet campaign	RTECS+ IUCLID- GESAMP- CPDB+ IRIS+	3	(3)	4	C M R	Very high acute toxicity Serious long term effects OEL-TWA: 0.001 mg/m3 IRIS: Carcinogen risk from inhalation calculated	C4
4-nitroso- morpholine	59-89-2		MEA S1 S3 S4 S9 Detected in ACCs Longannet campaign	RTECS+ IUCLID- GESAMP- CPDB+ IRIS-	2	(2)	(4)	C M	High acute toxicity Very high inhalation hazard Serious long term effects OEL-TWA: 0.001 mg/m3	B4
Nitrosamines (NOS)					3	(3)	4	C M R	High acute toxicity Very high inhalation hazard Serious long term effects OEL-TWA: 0.001 mg/m3	
1-nitro-piperazine	42499- 41-2		S4 S9	RTECS- IUCLID- GESAMP- CPDB- IRIS-	-	-	-	-	No data May well behave partly like piperazine and produce nitrosoamines in a nitrate rich environment. Potential A4	A3

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Degradation product	CAS.	Structure	Possible solvent origin	Data bases	Oral	Dermal	Inhal	Long term	Comment on human health hazard	Prio
N,N'- Dinitropiperazine	4164- 37-8		S4 S9	RTECS+ IUCLID- GESAMP- CPDB- IRIS-	No data	No data	No data	No data	No relevant data Two O-N=O groups. Could be reactive and a potential A4	A3
Dimethylnitramine	4164- 28-7		MEA S1 S3 S4 S9	RTECS+ IUCLID- GESAMP- CPDB+ IRIS-	1	No data	No data	C M	Serious long term effects	B3
Nitramines (NOS)					1	No data	No data	C M	May produce nitrosamines in a nitrate- rich environment	
Methylamine	74-89-5	H <sub>2</sub> N——	MEA S1 S3 S4 S9	RTECS+ IUCLID+ GESAMP+ CPDB- IRIS-	2	(2)	3	M		B3
Dimethylamine	124-40- 3	N H	MEA S1 S3 S4 S9	RTECS+ IUCLID+ GESAMP+ CPDB- IRIS+	2	0	3	M? S	May produce nitrosamines OEL: 3.5 mg/m3	B3
Ethylamine	75-04-7	H <sub>2</sub> N	MEA S1 S3 S4 S9	RTECS+ IUCLID+ GESAMP+ CPDB- IRIS-	2	2	1	-		B3

Degradation product	CAS.	Structure	Possible solvent origin	Data bases	Oral	Dermal	Inhal	Long term	Comment on human health hazard	Prio
Piperazine	110-85- 0	HNNH	S4 S9	RTECS+ IUCLID+ GESAMP- CPDB- IRIS-	2	0	2	(M) (S)	May produce nitrosamine OEL: 0.3 mg/m3	B4
Diethanolamine (DEA)	111-42- 2	Но ОН	MEA S3	RTECS+ IUCLID+ GESAMP+ CPDB- IRIS-	1	0	(0)	C M R	C, M, R: maybe not the compound itself. But will form nitrosoamine (CAS1116-54-7) with nitrites present	B4
Amines (NOS)					2	2	3	C M R	May produce nitrosamines OEL: 0.3 mg/m3	
Ammonia	7664- 41-7	NH3		RTECS+ IUCLID+ GESAMP+ CPDB- IRIS	1	(2)	3	M?	Health hazards well documented. OEL 18 mg/m3	CO
Formaldehyde	20-00-0	р н		RTECS+ IUCLID+ GESAMP- CPDB+ IRIS	2	2	4	C M S R?	Health hazards well documented. OEL 0.6 mg/m3	C3
Acetaldehyde	75-07-0			RTECS+ IUCLID+ GESAMP- CPDB+ IRIS	1	0	0	C M R S	Health hazards well documented OEL 45 mg/m3	C3



Degradation product	CAS.	Structure	Possible solvent origin	Data bases	Oral	Dermal	Inhal	Long term	Comment on human health hazard	Prio
Acetone	67-64-1	Ļ		RTECS+ IUCLID+ GESAMP+ CPDB- IRIS	0	0	0		Health hazards well documented OEL 295 mg/m3	C0
Formamide	75-12-7	0 <sup>NH</sup> 2		RTECS+ IUCLID+ GESAMP- CPDB- IRIS	0	0	1	R	Health hazards well documented OEL 18 mg/m3	C3

#### 4.2.2.2 Components of the emissions from the CO2 capture process

The emissions can be divided into four categories:

- Nitrosoamines
- Nitramines
- Amines
- Others (including aldehyde, organic acids etc)

#### **Nitrosoamines**

The nitrosoamines vary in their acute oral/dermal toxicity. Due to their N=O bond they all have the capacity to inflict lung damage. In cases where compounds do not have experimental data for inhalation toxicity it should be expected that they do have acute lung toxicity until proven otherwise. When examined or tested, these substances have been shown to be carcinogenic – either in humans or experimental animals with a classification of at least 2 according to IARC. Again, in cases where adequate data is not available it should be assumed that they are both carcinogenic and mutagenic until proven otherwise. As for reproductive effects only a few compounds have been tested – and shown to cause reproductive effects. Also for this endpoint it is suggested that any nitrosoamine is considered to have reproductive effects until proven otherwise through appropriate tests. Several compounds require metabolic activation and any *in vitro* toxicity testing must incorporate an appropriate system for test compound metabolism.

All the listed nitrosoamine compounds have at least some data available on both short term and long term health hazard. If we combine the available data a generic profile for nitrosoamines might be developed. We suggest that all nitrosoamine compounds are considered in a summary form by a generic term

*Nitrosoamines (NOS)* where NOS is an abbreviation for "not otherwise specified" We suggest that the hazard profile for nitrosoamines (NOS) is based on the worst case where data is available taking into the account that the group will include both aliphatic and aromatic compounds. The hazard profiles would then become as presented in Table 4.7.

#### <u>Nitramines</u>

Very limited data on mammalian or human toxicology was found for the nitramines. If we combine the compounds into a new generic profile based on worst case the hazard profile would become as presented in Table 4.7.

#### <u>Amines</u>

There are a range of amines identified as possible emissions. There is considerable variation in the availability of toxicological data for these compounds. Many compounds do not have data for long term effects (CMR). However, it is expected that such affects are common to many of these substances. Thus, one should expect that many of these compounds may become classified as CMRs when tested. It should also be noted that these compounds may produce nitrosamines if present in a nitrate/nitrite rich environment. A generic, worst case, profile has been developed as demonstrated in Table 4.7.

#### Other compounds

This group contains a wide range of chemical properties and a NOS-entry cannot be constructed. The compounds assumed to account for the highest release are shown in Table 4.7.

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#### 4.2.3 Provisional health risks of degradation products

The preceding table (Table 4.7) and considerations relate to the health hazards of the compounds. The risk analysis combines the intrinsic hazards of the compounds with the possible exposure scenario into e.g. exposure limit values. It is a relatively simple process to generate exposure limits for acute effects which occur after high exposure over a short time. However, setting exposure standards for low level exposure to compounds like carcinogens, mutagens and reprotoxins can be both time consuming and very difficult.

For the carbon capture process a risk analysis would require – for each compound:

- Estimated release, average and peak concentrations
- Estimated concentration in inhalable air at ground level
- Decomposition including biodegradation of compound
- Environmental conversions (e.g. amines to nitrosoamines)
- Bioaccumulation through food chain

This will assist the risk analyzer to determine the possible exposure scenario for the population in question.

For each of the most important endpoints (C, M and R) we would need a dose-response assessment – ie what is the expected increase of effect (C/M/R) at a certain exposure level. Developing such relationship for carcinogen is a prime aspect of the CPDB-database. As such information seldom is available for the complete set of chemicals (as in this list) a worst case compound would have to be used as a model.

Based on the input above one should be able to calculate excess number of incidents (of C/M/R) at a certain exposure level. It is then a governmental decision as to what level of excess incidents is accepted.

In the present case, as a first provisional approach, we could use the OEL divided by 100 as an indicator permissible exposure limit for the general population. The factor of 100 is rather arbitrary but should intentionally cover characteristics not encountered for work exposure limits:

- continuous exposure
- a wide age range
- a non-healthy population
- women at child-bearing age

Using such a factor for compounds identified for the TCM process we would arrive at the following provisional air limits as shown in Table 4.8.

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Table 4.8	Provisional ambient air limits at ground level, based on OEL-values presented in
	<i>Table 4.7.</i>

Compound	Ambient air limit (µg/m³)
Nitrosoamines (NOS)	0.01
Nitramines (NOS)	0.01
expected to convert to nitrosamines	
Amines (NOS)	3
Amines (NOS)	0.01
expected to convert to nitrosamines	
Ammonia	180
Formaldehyde	6

Some important issues are demonstrated:

- The nitrosamines may contribute to the health risk of the population even if their emission concentrations are small
- The possible conversion of amines to nitrosoamines should be carefully reviewed as this phenomena may change the overall risk assessment
- When considering formaldehyde it should be taken into account that the population already are exposed to this compound in several ways

Measured flue gas emission data are available for all these degradation products (e.g. Rokjær and Vang, 2009), but no measured or predicted data for actual ground levels exist. Therefore, the real risks of these products are not yet known. These assumptions made in Table 4.8 also show the needs for developing  $CO_2$  capture technologies which minimizes or eliminates the emissions of nitrosamines and products which may generate nitrosamines.

#### 4.3 Registration in REACH

All 27 degradation products were checked if they were pre-registered in REACH on the ECHA homepages (http://apps.echa.europa.eu/preregistered/pre-registered-sub.aspx). The results of Table 4.9 show that 17 of the degradation products were pre-registered in REACH, with latest registration dates ranging from 30.11.2010 to 31.5.2018. By these dates quality assured HE-data should be available for the pre-registered products for the following endpoints if these are chemicals produced in amounts  $\geq$ 10 tonnes/y:

Human health:

- Acute toxicity
- Mutagenicity/genotoxicity
- Reproduction toxicity
- Irritation/corrosion
- Sensitisation
- Repeated dose toxicity

Ecotoxicity:

- Acute toxicity to algae
- Acute toxicity to invertebrates
- Acute toxicity to fish
- Ready biodegradability
- Bioaccumulation

Table 4.9Pre-registered degradation products in REACH with latest date of<br/>registration. The products are separated in nitrosamines (blue), nitramines<br/>(pink) and amines/amides (green).

Degradation product	CAS	REACH	Registration date
N-nitrosodimethyl-amine	62-75-9	Yes	30.11.2010
4-nitroso-morpholine	59-89-2	No	
1-Nitrosopiperazine	5632-47-3	No	
N,N'-dinitrosopiperazine	140-79-4	Yes	30.11.2010
N-nitroso N'-aminoethyl piperazine	No CAS	No	
N-nitroso-diethanolamine	1116-54-7	No	
2-(methyl-nitrosoamino)- Ethanol	26921-68-6	No	
1-nitro-piperazine	42499-41-2	No	
N,N'-Dinitropiperazine	4164-37-8	Yes	31.05.2013
Dimethylnitramine	4164-28-7	No	
Methylamine	74-89-5	Yes	30.11.2010
Dimethylamine	124-40-3	Yes	30.11.2010
2-methyl-2-(methylamino)- 1-Propanol	27646-80-6	Yes	31.05.2018
Ethylamine	75-04-7	Yes	30.11.2010
Piperazine	110-85-0	Yes	30.11.2010
4-methyl-1-Piperazineethanol	5464-12-0	No	
4,4-dimethyl-2-Oxazolidinone	26654-39-7	No	
Diethanolamine (DEA)	111-42-2	Yes	30.11.2010
N-(2-hydroxyethyl)- Formamide (HEF)	693-06-1	Yes	31.05.2013
N-(2-hydroxy-ethyl)imidazole (HEI)	1615-14-1	Yes	30.11.2010
Hydroxyethyl oxazolidone (HEO)	3356-88-5	No	
1-hydroxyethyl-3-methyl imidazolidone	22455-69-2	No	
2-methylaminoethanol	109-83-1	Yes	30.11.2010
1,2-Ethanediol or ethyleneglycol (EG)	107-21-1	Yes	30.11.2010
N,N-dimethylethanolamine	108-01-0	Yes	30.11.2010
1,2 Ethylenediamine	107-15-3	Yes	30.11.2010
2,2'-[[2-[(2- hydroxyethyl)methylamino]ethyl]imino]bis- Ethanol (MTHEED)	187731-33-5	No	

#### 5 Conclusions

In this report we have described the formation of degradation products from amine-based post combustion  $CO_2$  capture, with emphasis on the degradation before emission to air.

The formation of degradation products for TCM solvents has not been fully quantified. There are also many degradation products that have not been identified yet. We are therefore not at present able to provide a detailed estimate of emissions for all TCM solvents. Most degradation products are however expected to fall within the categories given in Table 2.1.

Many of the unidentified degradation products are components with low volatility that are expected to have a very small contribution to the overall emissions.

We expect that most of the emissions will consist of the solvent itself and volatile degradation products such as ammonia, formaldehyde and methylamine. MEA degradation products include several linear and cyclic amines, but also nitramines and nitrosamines may be formed during degradation of solvent. However, several of the same degradation products may also be formed during degradation of other relevant TCM solvents, as well as several other products specific for solvent structures.

Nitrosamines have been detected experimentally in  $CO_2$  capture plants running with MEA as solvent. Two TCM solvents are likely to form more nitrosamine than MEA, while the others are likely to have a comparable or lower rate than formation than MEA.

A water-wash is expected to be efficient in removing medium volatility and low volatility degradation products.

An acid-wash is expected to be efficient in removing amine degradation products. An acid wash is not expected to be efficient in removing nitrosamines and nitramines.

The search for HE-information showed that much information is lacking, both with regard to environmental and health data. It seems that HE-data for volatile and non-volatile compounds are better covered than for medium volatile compounds.

The hazard related to the degradation products were mainly caused by the volatile aldehydes and amines. Some of these had PNEC values < 0.01 mg/L, corresponding to a EC50 or LC50 of < 10 mg/L However, all these products showed biodegradability in the range of 30-100 %, indicating that they will be degraded in biotic environments. Volatile amines also showed acute oral or dermal toxicity LD50 values < 2000 mg/k bw, and both aldehydes and amines were associated with positive or ambiguous mutagenicity/cytogenicity test results. Several of the volatile degradation products were also among the products with the highest reapeated dose (chronic) toxicity.

These data indicate that several of the degradation products associated with health and environmental hazard may escape the water wash due to their volatility.

Based on the data in Tables 3.5 to 3.8 the potential mutagenic effects of degradation products should receive some attention. A number of 12 products showed positive or ambiguous results in



Ames or cytogenetic tests. The many ambiguous test results may raise questions related to the quality of test performance. However, mutagenic and genotoxic effects should be related to the environmental concentrations of the products and the exposure conditions. The requirements for data related to real emission conditions are therefore required for risk analyses.

The variations in the data for volatile compounds also indicated a need for standardisation of exposure systems, since these compounds may escape the exposure systems if not kept totally closed.

The possible emissions or atmospheric generation of carcinogenic nitrosamines and nitramines from post combustion  $CO_2$  capture plants have received considerable attention. Only few health-related data from the nitrosamines identified in this study were found in public databases, and all of these have shown positive results in tests for mutagenicity/genotoxicity, as expected.

For provisional ecotoxicity hazard assessment (PNEC) some data were available for use, but for human toxicity hazard (DNEL), the material was very limited. The risk associated with these hazard values are difficult to predict, since they must be related to estimated environmental concentrations. In turn, these rely on a number of physical-chemical characteristics of the chemicals, as well as environmental and meteorological factors.

This present data search showed that the available HE information on degradation products from amines is still incomplete, and further data should be collected or obtained from confidential sources or from experimental studies for risk assessment studies of amines and their degradation products. Information from future REACH registration will also be of help for improving the data.

Potential health effects of 27 degradation products from five TCM-relevant solvents were evaluated by searches in the RTECS and GESAMP-EHS databases, with focus on potential nitrosamines, nitramine and amine/amide products. Data informations on several of the products were limited, but most the products with available mammal toxicity data could be considered to represent a possible environmental health hazard.

A provisional health risk evaluation of the 27 degradation products were conducted, with an OEL divided by 100 to represent a permissable exposure limit for the general population. This resulted in ambient air limits of 0.01 to  $180 \ \mu g/m^3$ , with nitrosamines, nitramines and amines converted to nitrosamines with the lowest limits. Based on these limits nitrosamines may contribute to the health risk of the population, although their emission concentration is small. However, the real risks can no be estimated before the fate of these compounds have been determined.

A search on the ECHA homepages showed that 15 of the 27 degradation products were preregistered in REACH, most of these with registration dates at the end of 2010. This means that improved HE-information for these will be available in near future.

As described in the report, the knowledge status of degradation products is better for MEA than for the other potential TCM-solvents, with better characterization of degradation products, and thus more HE-information available.

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## Appendix A – Possible nitrosamine and nitramine products from atmospheric degradation

Table A.1Theoretical atmospheric degradation products from amines, including name<br/>(if available), chemical formula, CAS no (if available) and atmospheric<br/>degradation time ( $\tau_{OH}$ ). Specific notes are made for the nitrosamines and<br/>nitramines with carcinogenic effects. All data collected from Bråten et al.<br/>(2009).

Degradation products	CAS.	Chemical formula	Comments
Formamide	75-12-7	H <sub>2</sub> NCHO	$\tau_{\rm OH}\!>3$ days
2-hydroxyacetamide	598-45-2	NH <sub>2</sub> C(=O)CH <sub>2</sub> OH	$\tau_{\rm OH}$ > 3 day
2-amino-2-oxo-peroxyacetylnitrate		H <sub>2</sub> NC(O)C(O)OONO <sub>2</sub>	
2-oxo-acetamide		H <sub>2</sub> NC(O)CHO	$\tau_{\rm OH}$ < 3 day
2-amino-peroxyacetyl-nitrate		H <sub>2</sub> NCH <sub>2</sub> C(O)OONO <sub>2</sub>	$\tau_{\rm OH}\!<\!3$ day
Methaneimine		HN=CH <sub>2</sub>	
Methaneimine Possible nitrosamines and nitramines	CAS.	HN=CH <sub>2</sub> Chemical formula	Comments
	CAS.		<b>Comments</b> Hydrogen abstraction from the amino group
Possible nitrosamines and nitramines	CAS.	Chemical formula	Hydrogen abstraction
Possible nitrosamines and nitramines 2-nitrosoamino-ethanol	CAS.	Chemical formula ON-NHCH <sub>2</sub> CH <sub>2</sub> -OH	Hydrogen abstraction

Degradation products	CAS no.	Chemical formula	Comments	
Acetamide	60-35-5	CH <sub>3</sub> C(O)NH <sub>2</sub>		
Hydroxyacetone	116-09-6	CH <sub>3</sub> C(O)CH <sub>2</sub> OH		
Hydroxylacetamide		CH <sub>2</sub> OCHC(O)NH <sub>2</sub>		
		(CH <sub>3</sub> ) <sub>2</sub> C(NH <sub>2</sub> )C(O)OONO		
Possible nitrosamines and nitramines	CAS no.	Chemical formula	Comments	
N-Nitrosoformamide	675141-02-3	CH <sub>3</sub> C(O)NHNO	Hydrogen abstraction	
N-Nitroformamide	51883-27-3	CH <sub>3</sub> C(O)NHNO <sub>2</sub>	from the amino group	

#### Table A.1 Theoretical atmospheric degradation products from amines (continued)

Degradation products	CAS no.	Chemical formula	Comments
Amide		(CH <sub>3</sub> )(CH <sub>2</sub> CH <sub>2</sub> OH)NCHO	$\tau_{\rm OH}$ > 3 days
Amide		CH <sub>3</sub> )(CH <sub>2</sub> OH)NCHO	$\tau_{\rm OH}$ > 3 days
PAN-like compound		(CH <sub>3</sub> )(CH <sub>2</sub> CH <sub>2</sub> OH)NCH <sub>2</sub> (O)OONO <sub>2</sub>	
PAN-like compound		(CH <sub>3</sub> )(CH <sub>2</sub> OH)NCH <sub>2</sub> (O)OONO <sub>2</sub>	
Amide		(CH <sub>3</sub> )(CH <sub>2</sub> CH <sub>2</sub> OH)NC(O)CH <sub>2</sub> OH	$\tau_{\rm OH}$ > 3 days
Amide		(CH <sub>3</sub> )(CH <sub>2</sub> OH)NC(O)CH <sub>2</sub> OH	$\tau_{\rm OH}$ > 3 days
<sup>A)</sup> PAN-like compound		(CH <sub>3</sub> )(CHOHCH <sub>2</sub> OH)NCH <sub>2</sub> C(O)OONO <sub>2</sub>	
<sup>A)</sup> PAN-like compound		(CH <sub>3</sub> )(CH <sub>2</sub> OH)NCHOHC(O)OONO <sub>2</sub>	
N-methylformamide	123-39-7	CH <sub>3</sub> NHCHO	
N-hydroxymethyl- formamide	13052- 19-2	(CH <sub>2</sub> OH)NHCHO	
N,N-diethanol- formamide		(CH <sub>2</sub> CH <sub>2</sub> OH) <sub>2</sub> NCHO	
N-methanol- N-ethanol- formamide		(CH <sub>2</sub> CH <sub>2</sub> OH)( CH <sub>2</sub> OH)NCHO	$\tau_{\rm OH}$ > 3 days

#### Table A.1 Theoretical atmospheric degradation products from amines (continued).

<sup>A)</sup> PAN, Peroxyacetyl nitrate

Possible nitrosamines and nitramines	CAS no.	Chemical formula	Comments
Nitrosamine		ONN(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> OH	
Nitramine		O <sub>2</sub> NN(CH <sub>3</sub> ) CH <sub>2</sub> CH <sub>2</sub> OH	From CH <sub>3</sub> N(CH <sub>2</sub> CH <sub>2</sub> OH)CH <sub>2</sub> CHOH
Nitrosamine		ONN(CH <sub>2</sub> CH <sub>2</sub> OH)CH <sub>2</sub> OH	radical
Nitramine		O <sub>2</sub> NN(CH <sub>2</sub> CH <sub>2</sub> OH)CH <sub>2</sub> OH	
Nitrosamine		ONN(CH <sub>3</sub> )CH <sub>2</sub> OH	
Nitrosamine		ONN(CH <sub>2</sub> OH) <sub>2</sub>	From
Nitramine		O <sub>2</sub> NN(CH <sub>3</sub> )CH <sub>2</sub> OH	CH <sub>3</sub> N(CH <sub>2</sub> CH <sub>2</sub> OH)ČH <sub>2</sub> CHOH radical
Nitramine		O <sub>2</sub> NN(CH <sub>2</sub> OH) <sub>2</sub>	
Nitrosamine		ONN(CH <sub>2</sub> CH <sub>2</sub> OH) <sub>2</sub> (fast photolysis during daytime)	From ĈH <sub>3</sub> N(CH <sub>2</sub> CH <sub>2</sub> OH)CH <sub>2</sub> CHOH
Nitramine		O <sub>2</sub> NN(CH <sub>2</sub> CH <sub>2</sub> OH) <sub>2</sub>	radical

#### Table A.1 Theoretical atmospheric degradation products from amines (continued).

Degradation products	CAS no.	Chemical formula	Comments
2-piperazone		CH <sub>2</sub> CH <sub>2</sub> NHCH <sub>2</sub> CO-NH	$\tau_{\rm OH}$ > 3 days
N,N'-1,2-ethanediylbis-formamide		CHONHCH <sub>2</sub> CH <sub>2</sub> NHCHO	$\tau_{\rm OH} > 3$ days
Amine/Amide/Aldehyde		H <sub>2</sub> NC(O)CH <sub>2</sub> NHCH <sub>2</sub> CHO	
Possible nitrosamines and nitramines	CAS no.	Chemical formula	Comments
Nitrosamine		ONNHC2CH2NHCH2CHO	
Nitramine		O2NNHC2CH2NHCH2CHO	

#### Table A.1 Theoretical atmospheric degradation products from amines (continued).

#### **Appendix B – Possible amine biodegradation products**

 Table B.1
 Common products from biodegradation of amines

Biodegradation products	CAS no.	Structure
Ammonia	7664-41-7	NH3
Acetaldehyde	75-07-0	Н <sub>3</sub> С—
Acetone	67-64-1	H <sub>3</sub> C CH <sub>3</sub>
Formaldehyde	50-00-0	H <sub>2</sub> C=O
Glycolic acid	79-14-1	НООН
Glyoxylic acid	298-12-4	
Lactic acid	50-21-5	HO O H <sub>3</sub> C OH
Malonate semialdehyde		HOHO
Ethanolamine (MEA)	141-43-5	H <sub>2</sub> N—OH
Piperazine	110-85-0	HNNH



Table B.1Continued

Biodegradation products	CAS no.	Structure
Pyruvate	113-24-6	H <sub>3</sub> C OH
Propionoic acid	6628-34-8	Н <sub>3</sub> С—ОН
Oxalic acid	144-62-7	о О НО ОН

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# Appendix C- List of degradation products for TCM solvents

Support on input to environmental discharges Evaluation of degradation components

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14 July 2010

List revised to match estimated emissions from plant

Degradation product	CAS.	Structure	dG solv	Ref./Comment
N-nitrosodimethylamine	62-75-9		-2.6(v)	Likely nitrosamine degradation product. May form in all TCM solvents. Detected in ACCs Longannet campaign
4-nitroso-morpholine	59-89-2		-4.4(v)	Detected in ACCs Longannet campaign. May form in MEA and solvent 3.
1-Nitrosopiperazine	5632-47- 3		-7.0(v)	Likely nitrosamine for TCM solvent 4 and 9.
N,N'-dinitrosopiperazine	140-79-4		-5.0(v)	Likely nitrosamine for TCM solvent 4 and 9
N-nitroso N'-aminoethyl piperazine	No CAS	N N NH2	-5.2(v)	Likely nitrosamine for TCM solvent 9
N-nitrosodiethanolamine	1116-54- 7	от и но по	-9.0(mv)	Detected in ACCs Longannet campaign. Likely for MEA and solvent 3.
2-(methylnitrosoamino)- Ethanol	26921- 68-6	N OH	-5.5(v)	May form in MEA and solvent 3
1-nitro-piperazine	42499- 41-2	HN N N	-8.0	Likely nitrosamine for TCM solvent 4 and 9.
N,N'- Dinitropiperazine	4164-37- 8		-3.9	Likely nitrosamine for TCM solvent 4 and 9.



Dimethylnitramine	4164-28- 7		-3.7	May form in all TCM solvents
Methylamine	74-89-5	H <sub>2</sub> N	V	May form in all TCM solvents
Dimethylamine	124-40-3	Z H	V	May form in all TCM solvents
2-methyl-2- (methylamino)- 1- Propanol	27646- 80-6	HO		May form in solvent 1
Ethylamine	75-04-7	H <sub>2</sub> N	V	May form in all TCM solvents
Piperazine	110-85-0	HNNH	-7.4	Solvent 4, may form in solvent 9
4-methyl-1- Piperazineethanol	5464-12- 0			May form in solvent 3
4,4-dimethyl-2- Oxazolidinone	26654- 39-7	NH O	-5.9	Expected for solvent 1
Diethanolamine (DEA)	111-42-2	HO N OH	-12.9	Expected for MEA and solvent 3
N-(2-hydroxyethyl)- Formamide (HEF)	693-06-1	HO	-11.6	Expected for MEA and solvent 3. Result of oxidative degradation. Expected to accumulate over time.
N-(2- hydroxyethyl)imidazole (HEI)	1615-14- 1	он	-14.6	Expected for MEA and solvent 3. Result of oxidatve degradation. Does to some extent accumulate over time.
Hydroxyethyl oxazolidone (HEO)	3356-88- 5	HONNO		May form in TCM solvent 3



1-hydroxyethyl-3- methyl imidazolidone	22455- 69-2	HO	May form in TCM solvent 3
2-methylaminoethanol	109-83- 1	н он	May form in MEA and TCM solvent 3
1,2-Ethanediol or ethyleneglycol (EG)	107-21- 1	но	May form in MEA and TCM solvent 3
N,N- dimethylethanolamine	108-01- 0	HONN	May form in TCM solvent 3
1,2 Ethylenediamine	107-15- 3	H <sub>2</sub> N NH <sub>2</sub>	Likely for TCM solvent 4 and 9
2,2'-[[2-[(2- hydroxyethyl)methyla mino]ethyl]imino]bis- Ethanol (MTHEED)	187731 -33-5	НООН	May form in TCM solvent 3

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# 7 Appendix D – Toxicity report on mammalian toxicology - human health hazard

# Introduction/background

The summary table condenses the results from the databases which have been examined. For classification and numerical rating the definitions used by GESAMP/EHS have been used. GESAMP is an organization for cooperation between several UN organizations (UNEP, FAO, UNESCO, IOC, WHO, WMO, IMO, IAEA). GESAMP/EHS was established in 1974 and have carried out detailed examination on roughly 3000 compounds and products carried at sea. The GESAMP classification is carried out by a team of international experts on chemistry, marine ecotoxicity and human health hazard assessment. The experts are invited by IMO (International Maritime Organization) on behalf of GESAMP. Their classification has been published as the GESAMP Composite list by IMO. The GESAMP/EHS review is based on public records as well as confidential company information. In some cases laboratory reports from the toxicity studies have been examined. The files supporting the decisions of the GESAMP/EHS group is located at IMO, London, UK.

Although the GESAMP/EHS profile is generated in order to regulate the safe transport of chemicals at sea, the information on human can be used also for other purposes.

# **Principles of evaluation**

In the present project exposure to humans may occur in an occupational setting or as a result of chemicals being dispersed to the neighborhood of the production plant. Any controversy as to exposure limits etc will most probably be focused on the neighborhood environment. Thus, acute oral and dermal toxicity will play a minor role in the final overall assessment. Acute (4 hours) inhalation data will of course be important in any setting where atmospheric exposure is the prime source. However, acute short term exposure at relatively high concentrations may not be a good indicator of health hazards which may occur after low level and long term exposure.

At low level and long term exposure the following health hazards will be of prime interest when regulations are set for permissible exposure to population at or near a plant:

- Carcinogenicity (C)
- Mutagenicity (M)
- Reproductive effects (R)
- Sensitization, primarily by inhalation (S)

The overall assessment of these substances has been suggested in the "comments" and "prio" columns. The two columns taken together should offer some advice to the future development of risk analysis scenarios as well as limits for acceptable atmospheric release and resulting environmental exposure to humans.

The "Prio" column summarizes two indicators – a letter and a number. The letter is an abbreviated assessment of the data which have been found in the available databases:

А	Inadequate data for assessment of hazard
В	Inadequate data for assessment of hazard. Further data may be found in e.g.
	company records
С	Adequate data for hazard evaluation

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The number is a provisional estimation of long term health risk relative to air contamination. The numerical value reflects data regarding important long term health issues:

С	Shown to induce or increase cancer in animals or man
М	Shown to cause increased incidence of permanent changes in the amount or structure of the genetic material
R	Shown to cause adverse effects on reproductive ability or capacity, or the development of offspring
S	Shown to be a sensitizer (skin or respiratory)

A summary evaluation of these risks is then given a numerical value:

0	None or very low long term health risk
1	Low long term health risk
2	Medium long term health risk
3	High long term health risk
4	Very high long term health risk

# Components of the emissions from the CO2 capture process

The emissions can be divided into four categories:

- Nitrosoamines
- Nitramines
- Amines
- Others (including aldehyde, organic acids etc)

# Nitrosoamines

The nitrosoamines vary in their acute oral/dermal toxicity. Due to their N=O bond they all have the capacity to inflict lung damage. In cases where compounds do not have experimental data for inhalation toxicity it should be expected that they do have acute lung toxicity until proven otherwise. When examined or tested, these substances have been shown to be carcinogenic – either in humans or experimental animals with a classification of at least 2 according to IARC. Again, in cases where adequate data is not available it should be assumed that they are both carcinogenic and mutagenic until proven otherwise. As for reproductive effects only a few compounds have been tested – and shown to cause reproductive effects. Also for this endpoint it is suggested that any nitrosoamine is considered to have reproductive effects until proven otherwise through appropriate tests. Several compounds require metabolic activation and any *in vitro* toxicity testing must incorporate an appropriate system for test compound metabolism.

All the listed nitrosoamine compounds have at least some data available on both short term and long term health hazard. If we combine the available data a generic profile for nitrosoamines might be developed. We suggest that all nitrosoamine compounds are considered in a summary form by a generic term

Nitrosoamines (NOS) where NOS is an abbreviation for "not otherwise specified"



We suggest that the hazard profile for nitrosoamines (NOS) is based on the worst case where data is available taking into the account that the group will include both aliphatic and aromatic compounds. The hazard profile would then become:

Name	CAS	Oral	Percutaneous (Dermal)	Inhalation	Long term	Comment
N-	62-75-	3	(3)	4	С	Very high
nitrosodimethylamine	9				Μ	acute
					R	toxicity
						OEL-
						TWA:
						0.001
						mg/m3
4-nitrosomorpholine	59-89-	2	(2)	4	C	Very high
	2				Μ	acute
						toxicity
						OEL-
						TWA:
						0.001
						mg/m3
Nitrosoamines (NOS)		3	(3)	4	С	Very high
					M	acute
					R	toxicity
						OEL-
						TWA:
						0.001
						mg/m3

# Nitramines

Very limited data on mammalian or human toxicology was found for the nitramines. If we combine the compounds into a new generic profile based on worst case the hazard profile would become:

Name	CAS	Oral	Percutaneous (Dermal)	Inhalation	Long term	Comment
1-nitro-piperazine	42499- 41-2	-	-	_	-	May produce nitrosamine in a nitrate rich environment
N,N'- dinitropiperazine	4164- 37-8	-	-	-	-	
Dimethylnitramine	4164- 28-7	1	-	-	C M	



Nitramines (NOS)	 1	-	-	С	May
				M	produce
					nitrosamine
					in a nitrate
					rich
					environment

# Amines

There are a range of amines identified as possible emissions. There is considerable variation in the availability of toxicological data for these compounds. Many compounds do not have data for long term effects (CMR). However, it is expected that such affects are common to many of these substances. Thus, one should expect that many of these compounds may become classified as CMRs when tested. It should also be noted that these compounds may produce nitrosamines if present in a nitrate/nitrite rich environment. A generic, worst case, profile has been developed as demonstrated below:

Name	CAS	Oral	Percutaneous	Inhalation	Long	Comment
	74.00		(Dermal)	2	term	
Methylamine	74-89-	2	(2)	3	Μ	
	5					
Dimethylamine	124-	2	0	3	M?	May
	40-3				S	produce
						nitrosamine
						OEL: 3.5
						mg/m3
Ethylamine	75-04-	2	2	1		
	7					
Piperazine	110-	2	0	2	(M)	May
1	85-0				(S)	produce
						nitrosamine
						OEL: 0.3
						mg/m3
Diethanolamine	111-	1	0	0	С	
(DEA)	42-2				Μ	
					R	
Amines (NOS)		2	2	3	С	May
					M	produce
					R	nitrosamine
						OEL: 0.3
						mg/m3



# Other compounds

This group contains a wide range of chemical properties and a NOS-entry cannot be constructed. The compounds assumed to account for the highest release is:

Name	CAS	Oral	Percutaneous	Inhalation	Long	Comment
			(Dermal)		term	
Ammonia	7664-	1	(2)	3	M?	OEL: 18
	41-7					Mg/m3
Formaldehyde	20-00-	2	2	4	С	OEL: 0.6
	0				Μ	mg/m3
					S	_
					R?	
Acetaldehyde	75-07-	1	0	0	С	OEL: 45
	0				Μ	mg/m3
					R	-
					S	
Acetone	67-64-	0	0	0	-	OEL: 295
	1					Mg/m3
Formamide	75-12-	0	0	1	R	OEL: 18
	7					Mg/m3

# Comments on a provisional risk analysis

The preceding tables and considerations relate to the health hazards of the compounds. The risk analysis combines the intrinsic hazards of the compounds with the possible exposure scenario into e.g. exposure limit values. It is a relatively simple process to generate exposure limits for acute effects which occur after high exposure over a short time. However, setting exposure standards for low level exposure to compounds like carcinogens, mutagens and reprotoxins can be both time consuming and very difficult.

For the carbon capture process a risk analysis would require – for each compound:

- Estimated release, average and peak concentrations
- Estimated concentration in inhalable air at ground level
- Decomposition including biodegradation of compound
- Environmental conversions (e.g. amines to nitrosoamines)
- Bioaccumulation through food chain

This will assist the risk analyzer to determine the possible exposure scenario for the population in question.

For each of the relevant endpoints (C, M and R) we would need a dose-response assessment – ie what is the expected increase of effect (C/M/R) at a certain exposure level. Developing such relationship for carcinogen is a prime aspect of the CPDB-database. As such information seldom is available for the complete set of chemicals (as in this list) a worst case compound would have to be used as a model.

Based on the input above one should be able to calculate excess number of incidents (of C/M/R) at a certain exposure level. It is then a governmental decision as to what level of excess incidents is accepted.



In the present case, as a first provisional approach, we could use the OEL divided by 100 as an indicator permissible exposure limit for the general population. The factor of 100 is rather arbitrary but should intentionally cover characteristics not encountered for work exposure limits:

- continuous exposure
- a wide age range
- a non-healthy population
- women at child-bearing age

Using such a factor for compounds identified for the CCM process we would arrive at the following provisional air limits at ground level:

Compound	Ambient air limit (µg/m <sup>3</sup> )
Nitrosoamines (NOS)	0.01
Nitramines (NOS)	0.01
expected to convert to nitrosamines	
Amines (NOS)	3
Amines (NOS)	0.01
expected to convert to nitrosamines	
Ammonia	180
Formaldehyde	6

The table above demonstrates some important issues:

- The nitrosamines may contribute very significantly to the health risk of the population although their emission concentration is small
- The possible conversion of amines to nitrosoamines should be carefully reviewed as this phenomena may change the overall risk assessment
- When considering formaldehyde it should be taken into account that the population already are exposed to this compound in several ways

# **()** SINTEF

# Appendix E – Summaries of health-related data of degradation products related to TCM solvent emissions

Degradation product	CAS.	Structure	Ref./Comment	Data bases	Oral	Dermal	Inhal	Long term	Comment on human health hazard	Prio
N-nitrosodimethyl- amine	62-75-9		Likely nitrosamine degradation product. May form in most solvents. Detected in ACCs Longannet campaign	RTECS+ IUCLID- GESAMP- CPDB+ IRIS+	3	(3)	4	C M R	Very high acute toxicity Serious long term effects OEL: 0.001 mg/m3 IRIS: Carcinogen risk from inhalation calculated	C4
4-nitroso- morpholine	59-89-2		Detected in ACCs Longannet campaign. May form in most alkanolamine solvents.	RTECS+ IUCLID- GESAMP- CPDB+ IRIS-	2	(2)	(4)	C M	High acute toxicity Very high inhalation hazard Serious long term effects OEL: 0.001 mg/m3	B4
1-Nitrosopiperazine	5632- 47-3	HNNNN	Likely nitrosamine for TCM solvent 4 and 9.	RTECS+ IUCLID- GESAMP- CPDB+ IRIS-	0	-	-	C M	Remarkable low oral toxicity – <u>questionable</u> ! Serious long term effects	B4
N,N'- dinitrosopiperazine	140-79- 4		Likely nitrosamine for TCM solvent 4 and 9	RTECS+ IUCLID- GESAMP- CPDB+ IRIS-	2	3	-	C M R	High acute toxicity Expect inhalation hazard Serious long term effects	C4



Degradation product	CAS.	Structure	Ref./Comment	Data bases	Oral	Dermal	Inhal	Long term	Comment on human health hazard	Prio
N-nitroso N'- aminoethyl piperazine	No CAS	о N — N NH2	Likely nitrosamine for TCM solvent 9	RTECS- IUCLID- GESAMP- CPDB- IRIS-	-	-	-	(C) (M) (R)	Not found in any of the databases. Searched with several varieties of nomenclature. A second search for CAS# should be done. <i>Serious long</i> <i>term effects is to be</i> <i>expected.</i>	B4
N-nitroso- diethanolamine	1116- 54-7	ол и Но И ОН	Detected in ACCs Longannet campaign	RTECS+ IUCLID- GESAMP- CPDB+ IRIS+	0	(0)	-	C M (R)	Non-toxic by oral or dermal route. No data on reproductive effects <i>Serious long term effects</i> OEL: 0.001 mg/m3 IRIS on oral intake	C4
2-(methyl- nitrosoamino)- Ethanol	26921- 68-6	N OH	May form in some TMC solvents	RTECS+ IUCLID- GESAMP- CPDB+ IRIS-	-	-	-	C M (R)	No data on acute effects No data on reproductive effects <i>Serious long term effects</i>	B4
1-nitro-piperazine	42499- 41-2	HR R R R R R R R R R R R R R R R R R R		RTECS- IUCLID- GESAMP- CPDB- IRIS-	-	-	-	-	No data May well behave partly like piperazine and produce nitrosoamines in a nitrate rich environment. Potential A4	A3



Degradation product	CAS.	Structure	Ref./Comment	Data bases	Oral	Dermal	Inhal	Long term	Comment on human health hazard	Prio
N,N'- Dinitropiperazine	4164- 37-8			RTECS+ IUCLID- GESAMP- CPDB- IRIS-	-	-	-	-	No relevant data Two O-N=O groups. <i>Could be reactive and a</i> <i>potential A4</i>	A3
Dimethylnitramine	4164- 28-7			RTECS+ IUCLID- GESAMP- CPDB+ IRIS-	1	-	-	C M	Serious long term effects	B3
Methylamine	74-89-5	H <sub>2</sub> N		RTECS+ IUCLID+ GESAMP+ CPDB- IRIS-	2	(2)	3	М	Moderate acute toxicity. Serious long term effects OEL: 13 mg/m3 (RTECS)	B3
Dimethylamine	124-40- 3	ΞI		RTECS+ IUCLID+ GESAMP+ CPDB- IRIS+	2	0	3	M? S	Moderate acute toxicity OEL: 3.5 mg/m3 IRIS file withdrawn In presence of nitrous acid may form nitroso- dimethylamine (CAS62- 75-9). If such conditions exist then long term serious effects should be anticipated	B3
2-methyl-2- (methylamino)- 1- Propanol	27646- 80-6	HO		RTECS- IUCLID- GESAMP- CPDB- IRIS-	-	-	-	-	No data	A3



Degradation product	CAS.	Structure	Ref./Comment	Data bases	Oral	Dermal	Inhal	Long term	Comment on human health hazard	Prio
Ethylamine	75-04-7	H <sub>2</sub> N		RTECS+ IUCLID+ GESAMP+ CPDB- IRIS-	2	2	1	-	Moderate acute toxicity IUCLID: Tested for M negative. Not tested for C or R OEL: 18 mg/m3	B3
Piperazine	110-85- 0	HNNH	This is potential degradation product, in addition to being solvent	RTECS+ IUCLID+ GESAMP- CPDB- IRIS-	1	0	2	(M) (S)	Moderate acute toxicity OEL: 0.3 mg/m3 C-lungadenoma when coexposure with nitrite. In environment with nitrite or nitrates the respective nitrosoamine might be produced. Expect C, M and R as long term serious health effects.	B4
1,4 dimethyl- piperazine	106-58- 1	N		RTECS+ IUCLID- GESAMP- CPDB- IRIS-	-	0	-	-	Very little data Low dermal acute is not a good indicator for other acute tox	A3
4-methyl-1- Piperazineethanol	5464- 12-0	HO		RTECS- IUCLID- GESAMP- CPDB- IRIS-	-	-	-	-	No data	A2



Degradation product	CAS.	Structure	Ref./Comment	Data bases	Oral	Dermal	Inhal	Long term	Comment on human health hazard	Prio
Oxazolidine	497-25- 6		Certain degradation product in MEA	RTECS+ IUCLID- GESAMP- CPDB- IRIS-	-	-	-	(C)	RTECS skin cancer equivocal	A2
4,4-dimethyl-2- Oxazolidinone	26654- 39-7	NH O	Expected for 1 TCM solvent	RTECS- IUCLID- GESAMP- CPDB- IRIS-	-	-	-	-	No data	A2
4-(2-hydroxyethyl)- 2-Piperazinone	23936- 04-1	O N H		RTECS- IUCLID- GESAMP- CPDB- IRIS-	-	-	-	-	No data	A2
1-(2 hydroxyethyl)- 2-imidazolidinone (HEIA)	3699- 54-5	но		RTECS- IUCLID- GESAMP- CPDB- IRIS-	-	-	-	-	No data	A2
3,4,4-trimethyl oxazolidin-2-one	15833- 17-7			RTECS- IUCLID- GESAMP- CPDB- IRIS-	-	-	-	-	No data	A2



Degradation product	CAS.	Structure	Ref./Comment	Data bases	Oral	Dermal	Inhal	Long term	Comment on human health hazard	Prio
Diethanolamine (DEA)	111-42- 2	но он Н		RTECS+ IUCLID+ GESAMP+ CPDB- IRIS-	1	0	(0)	C M R	C, M, R: maybe not the compound itself. But will form nitrosoamine (CAS1116-54-7) with nitrites present	B4
N-(2-hydroxyethyl)- acetamide(HEA)	142-26- 7	HO HO	Result of oxidative degradation. Expected to accumulate over time.	RTECS+ IUCLID- GESAMP- CPDB- IRIS-	0	0	-	-		B3
N-(2-hydroxyethyl)- Formamide (HEF)	693-06- 1	HO	Result of oxidative degradation. Expected to accumulate over time.	RTECS- IUCLID- GESAMP- CPDB- IRIS-	-	-	-	-	No data	B3
N-(2-hydroxy- ethyl)imidazole (HEI)	1615- 14-1	Л ОН	Result of oxidatve degradation. Does to some extent accumulate over time.	RTECS- IUCLID- GESAMP- CPDB- IRIS-	-	-	-	-	No data	A2
(2-hydroxyethyl)- ethylenediamine, HEED	111-41- 1	HONH2 H	Result of thermal degradation. Transient degradation product.	RTECS+ IUCLID+ GESAMP+ CPDB- IRIS-	0	0	0	(M) R S	Low acute toxicity. Serious long term toxicity	B3



Degradation product	CAS.	Structure	Ref./Comment	Data bases	Oral	Dermal	Inhal	Long term	Comment on human health hazard	Prio
N,N-Bis(2-hydroxy- ethyl)glycine	150-25- 4	Но		RTECS+ IUCLID- GESAMP- CPDB- IRIS-	-	_	-	-	No relevant data. <i>Low ip tox – can assume</i> <i>low acute toxicity.</i>	A2

# Compounds on the emission application which was not initially considered

Compound	CAS.	Structure	Ref./Comment	Data bases	Oral	Dermal	Inhal	Long term	Comment on human health hazard	Prio
Ammonia	7664- 41-7	NH3		RTECS+ IUCLID+ GESAMP+ CPDB- IRIS	1	(2)	3	M?	Health hazards well documented. OEL 18 mg/m3	CO
Formaldehyde	50-00-0	U H H		RTECS+ IUCLID+ GESAMP- CPDB+ IRIS	2	2	4	C M S R?	Health hazards well documented. OEL 0.6 mg/m3	C3
Acetaldehyde	75-07-0	~O		RTECS+ IUCLID+ GESAMP- CPDB+ IRIS	1	0	0	C M R S	Health hazards well documented OEL 45 mg/m3	C3
Acetone	67-64-1	, or the second		RTECS+ IUCLID+ GESAMP+ CPDB- IRIS	0	0	0		Health hazards well documented OEL 295 mg/m3	C0
Formamide	75-12-7	0 NH2		RTECS+ IUCLID+ GESAMP- CPDB- IRIS	0	0	1	R	Health hazards well documented OEL 18 mg/m3	C3
Acetamide	60-35-5	NH <sub>2</sub>		RTECS+ IUCLID+ GESAMP- CPDB+ IRIS	0	-	-	C M R	Long term effects well documented No data for dermal/inhalation OEL 25 mg/m3	C3



Compound	CAS.	Structure	Ref./Comment	Data bases	Oral	Dermal	Inhal	Long term	Comment on human health hazard	Prio
1,2- ethylenediamine	107-15- 3	H <sub>2</sub> N NH <sub>2</sub>		RTECS+ IUCLID+ GESAMP+ CPDB- IRIS	1	2	1	R M? S	Has tested negative for C The M is questionable OEL 25 mg/m3	B2
Diethylamine	109-89- 7			RTECS+ IUCLID+ GESAMP+ CPDB- IRIS	1	2	3		RTECS and IUCLID differs on M assessment OEL 30 mg/m3	B2
1-Butanamine	109-73- 9	NH <sub>2</sub>		RTECS+ IUCLID+ GESAMP+ CPDB- IRIS	2	2	3		OEL: 15 mg/m3	C2
Dibutylamine	111-92- 2	~~~~ <sup>H</sup> ~~~~		RTECS+ IUCLID+ GESAMP+ CPDB- IRIS	2	2	3		OEL: 26 mg/m3	C2
N-methylethanamine	624-78- 2	H N N N N N N N N N N N N N N N N N N N		RTECS- IUCLID- GESAMP- CPDB- IRIS	-	-	-		No data found. By comparing with other alkane amines a long term health hazard is not expected	B2
N-methyl 1- butanamine	110-68- 9	Z H		RTECS+ IUCLID- GESAMP- CPDB- IRIS	1	1	(2)		Limited dataavailable	B2
N-ethyl 1- butanamine	13360- 63-9	H N		RTECS+ IUCLID- GESAMP+ CPDB- IRIS	1	1	2		Limited data available	B2



Compound	CAS.	Structure	Ref./Comment	Data bases	Oral	Dermal	Inhal	Long term	Comment on human health hazard	Prio
1-Propanamine	107-10- 8	NH <sub>2</sub>		RTECS+ IUCLID- GESAMP+ CPDB- IRIS	2	2	3		No data on long term exposure OEL (STEL) 12 mg/m3	B2
Dipropylamine	142-84- 7	H N		RTECS+ IUCLID+ GESAMP+ CPDB- IRIS	2	2	2		No data on long term exposure	B2
2,2'-[[2-[(2- hydroxyethyl)meth ylamino]ethyl]imin o]bis- Ethanol (MTHEED)	187731 -33-5	HONOH		RTECS- IUCLID- GESAMP- CPDB- IRIS	-	-	-		No data	A1
1,2-ethanediol Etylenglykol (EG)	107-21- 1	но		RTECS+ IUCLID - sjekk GESAMP+ CPDB+ IRIS	(1)	(1)	(1)	R		C2
N,N.dimetyletanola min	108-01- 0	HONN		RTECS+ IUCLID+ GESAMP+ CPDB+ IRIS	1	1	2	S	Tested for C and R – negative. OEL 36 mg/m3	C2
MMEA / Monometyletanola mine 2-metylaminetanol	109-83- 1	NHOH		RTECS+ IUCLID+ GESAMP- CPDB- IRIS	1	1	(1)		OEL 9.4 mg/m3	C2



Compound	CAS.	Structure	<b>Ref./Comment</b>	Data bases	Oral	Dermal	Inhal	Long term	Comment on human health hazard	Prio
1-hydroxyethyl-3- methyl imidazolidone	22455- 69-2	HONN		RTECS- IUCLID- GESAM- CPDB- IRIS	-	-	-	-	No data	A2
Hydroksyetyl oksazolidin (HEO)	3356- 88-5			RTECS+ IUCLID- GESAMP- CPDB- IRIS	-	-	-	-	N odata	A2
Maursyre Formic acid	64-18-6			RTECS+ IUCLID+ GESAMP+ CPDB- IRIS	1	(1)	2	-	OEL: 9 mg/m3	CO
Eddiksyre Acetic acid	64-19-7			RTECS+ IUCLID+ GESAMP+ CPDB- IRIS	1	1	1	-	OEL 25 mg/m3	C0
Butansyre Butyrin acid (smørsyre)	107-92- 6			RTECS+ IUCLID+ GESAMP+ CPDB- IRIS	1	2	0	-		C0
Propionsyre Propionic acid (Fettsyre)	79-09-4			RTECS+ IUCLID+ GESAMP+ CPDB- IRIS	0	2	(3)			C0
DEA / Dietanolamin	111-42- 2	НО ОН		RTECS IUCLID GESAMP CPDB- IRIS	1	0	(0)	R		B2



Appendix F – Hazard Summary Sheets for degradation products from TCM-relevant solvents

Chemical hazard summary sheet	
Tore Syversen	

CAS - No.	Name
Not known	N-nitroso N'-aminoethyl piperazine

EU-Risk phrases	
<b>Comments on chemical</b>	
Comments on evaluation	
GESAMP/EHS file	No
RTECS file	No
IUCLID file	No
REACH file	
Other sources	•

No.	CAS - No.	chemical name	remark
1			
2			

#### Column C1: Oral Toxicity

0: >200	00 1: 300-20	00 2: 50-3	00 3: 5-50	4: <5 mg/kg bw
Study no.	rating based on this study	LD <sub>50</sub> value	animal species	Source or comment
1				
2				
3				

 Column C2: Percutaneous Toxicity

 0: >2000
 1: 1000-2000
 2: 200-1000
 3. 50-200
 4: <50</td>
 mg/kg bw

Study no.	rating based on this study	LD <sub>50</sub> value	animal species	Source or comment
1				
2				
3				

# Column C3: Inhalation Toxicity

0: >20	1: 10-20	2: 2-10 3	: 0.5-2 4:	<0.5 mg/l (4hrs)
Study	rating based on	LC50 value	animal	Details, remarks, please indicate exposure time (hrs)
no.	this study	exp. time	species	
1				
2				
3				

Chemical hazard summary sheet	
Tore Syversen	

0: non-irritating 1: Mildly irritating 2: Irritating 3: Severely irritating or corrosive

3A: Corros	ive >1 hr-4 hr	3B: Corrosive >3 min < 1 hr	3C: Corrosive < 3min
study no.	proposed rating	source / kind of study / animal	species
1			
2			
3			

#### Column D2: Eye Irritation / Corrosion

0: Not irrita	ating 1: Mildl	ly irritating 2: Irritating 3: Severely irritating with irreversible corneal injury
study no.	proposed rating	source / kind of study / animal species
1		
2		
3		

# Column D3: Other long term effects (indicate by appropriate letter in box)

Carcinogenic - C	(C)	Aspiration haz A		Neurotoxic - N	
Lung injury - L		Reprotoxic – R	R	Immunotoxic - I	
Mutagenic - M	(M)	Photosensitizer - P		Sensitizing - S	
<b>Source/comment:</b> CMR: analogy with		rosoamines			

# <u>Remarks</u>

ACC2

Not found in any of the databases. Searched with several varieties of nomenclature. A second search for CAS# should be done. *Serious long term effects is to be expected.* 

C1	C2	C3	D1	D2	D3	Date

Chemical hazard summary sheet	
Tore Syversen	

CAS - No.	Name	
55-18-5	N-nitroso-diethylamine	

EU-Risk phrases	
<b>Comments on chemical</b>	
<b>Comments on evaluation</b>	
GESAMP/EHS file	No
RTECS file	IA3500000 Update: 200911
IUCLID file	
REACH file	
Other sources	•

No.	CAS - No.	chemical name	remark
1			
2			

# Column C1: Oral Toxicity

0: >200	00 1: 300-20	2: 50-3	00 3: 5-50	4: <5 mg/kg bw
Study no.	rating based on this study	LD <sub>50</sub> value	animal species	Source or comment
1	2	220	Rat	RTECS
2	2	200	Mouse	RTECS
3	2	250	Guinea	RTECS
			pig	

# Column C2: Percutaneous Toxicity

0: >200	0: >2000 1: 1000-2000 2: 200-1000 3. 50-200 4: <50 mg/kg bw						
Study	rating based on	LD <sub>50</sub> value	animal	Source or comment			
no.	this study		species				
1	3	195	Rat	RTECS			
2	2	232	Hamster				
3							

# Column C3: Inhalation Toxicity

0: >20	1: 10-20	2: 2-10 3	: 0.5-2 4:	<0.5 mg/l (4hrs)
Study	rating based on	LC50 value	animal	Details, remarks, please indicate exposure time (hrs)
no.	this study	exp. time	species	
1				
2				
3				

Chemical hazard summary sheet	
Tore Syversen	

0: non-irritating 1: Mildly irritating 2: Irritating 3: Severely irritating or corrosive

3A: Corros	ive $>1$ hr-4 hr 3	BB: Corrosive $>3 \min < 1 hr$	3C: Corrosive < 3min
study no.	proposed rating	source / kind of study / animal sp	ecies
1			
2			
3			

#### **Column D2: Eye Irritation / Corrosion**

0: Not irrita	ating 1: Mildl	y irritating 2: Irritating 3: Severely irritating with irreversible corneal injury
study no.	proposed rating	source / kind of study / animal species
1		
2		
3		

# Column D3: Other long term effects (indicate by appropriate letter in box)

Carcinogenic - C	С	Aspiration haz A		Neurotoxic - N			
Lung injury - L		Reprotoxic – R	R	Immunotoxic - I			
Mutagenic - M	Μ	Photosensitizer - P		Sensitizing - S			
Source/comment:							
C: RTECS many studies; liver, kidney, respiratory							

R: RTECS many studies; fetotoxic and abnormalities

M: RTECS many studies

# <u>Remarks</u>

IARC: Animal suffient, human no adequate data. Group 2A (1987)
OEL: Austria/Switzerland: 0.001-0.0025 mg/m3 (2006)

C1	C2	C3	D1	D2	D3	Date

Chemical hazard summary sheet	
Tore Syversen	

CAS - No.	Name
59-89-2	4-nitroso-morpholine

EU-Risk phrases	
<b>Comments on chemical</b>	
<b>Comments on evaluation</b>	
GESAMP/EHS file	No
RTECS file	QE7525000 Update: 200908
IUCLID file	No
<b>REACH file</b>	
Other sources	• CPDB+
	• IRIS-

No.	CAS - No.	chemical name	remark
1			
2			

# Column C1: Oral Toxicity

0: >200	00 1: 300-20	00 2: 50-3	00 3: 5-50	4: <5 mg/kg bw
Study	rating based on	LD <sub>50</sub> value	animal	Source or comment
no.	this study		species	
1	2	282	Rat	RTECS
2	1	956	Hamster	RTECS
3				

# Column C2: Percutaneous Toxicity

0: >200	0 1: 1000-20	00 2: 200-1	000 3. 50-20	0 4: <50 mg/kg bw
Study	rating based on	LD50 value	animal	Source or comment
no.	this study		species	
1	(2)	170	Rat	RTECS. Subcutaneous dose
2				
3				

# Column C3: Inhalation Toxicity

0: > 20	1: 10-20	2: 2-10 3	3: 0.5-2 4:	<0.5 mg/l (4hrs)
Study	rating based on	LC50 value	animal	Details, remarks, please indicate exposure time (hrs)
no.	this study	exp. time	species	
1	4	1	Mouse	10 minute exposure
2				
3				

Chemical hazard summary sheet	
Tore Syversen	

0: non-irritating 1: Mildly irritating 2: Irritating 3: Severely irritating or corrosive

3A: Corrosi	1  ve > 1  hr - 4  hr = 3	B: Corrosive >3 min < 1 hr 3C: Corrosive < 3min
study no.	proposed rating	source / kind of study / animal species
1		
2		
3		

 Column D2: Eye Irritation / Corrosion

 0: Not irritating
 1: Mildly irritating
 2: Irritating
 3: Severely irritating with irreversible corneal injury

study no.	proposed rating	source / kind of study / animal species
1		
2		
3		

#### Column D3: Other long term effects (indicate by appropriate letter in box)

Carcinogenic - C	С	Aspiration haz A	Neurotoxic - N	
Lung injury - L		Reprotoxic – R	Immunotoxic - I	
Mutagenic - M	Μ	Photosensitizer - P	Sensitizing - S	
Source/comment:				
C: RTECS many reports; liver, GI, respiratory				
M: RTECS many reports				

#### **Remarks**

IARC: Animal sufficient, human not adequate. Group 2B. Classified in 1987
OEL: Austria and Switzerland: 0.001-0,0025 mg/m3 classified in 2006
NTP: Reasonably anticipated to be a human carcinogen (2004)
ACC2
High acute toxicity
Very high inhalation hazard
No data on reproductive effects
Serious long term effects
OEL: 0.001 mg/m3

C1	C2	C3	D1	D2	D3	Date

Chemical hazard summary sheet	
Tore Syversen	

CAS - No.	Name
62-75-9	N-nitrosodimethylamine

EU-Risk phrases	
<b>Comments on chemical</b>	
<b>Comments on evaluation</b>	
GESAMP/EHS file	No
RTECS file	IQ0525000 Update: 20911
IUCLID file	No
<b>REACH file</b>	
Other sources	• IRIS+
	• CPDB+

I	No.	CAS - No.	chemical name	remark
	1			
I	2			

# Column C1: Oral Toxicity

0: >200	0: >2000 1: 300-2000 2: 50-300 3: 5-50 4: <5 mg/kg bw						
Study	rating based on	LD <sub>50</sub> value	animal	Source or comment			
no.	this study		species				
1	3	37	Rat	RTECS			
2	3	28	Hamster	RTECS			
3							

# Column C2: Percutaneous Toxicity

0: >200	0: >2000 1: 1000-200 2: 200-1000 3. 50-200 4: <50 mg/kg bw						
Study	rating based on	LD50 value	animal	Source or comment			
no.	this study		species				
1	(3)	15	Rat	RTECS Russian data. Subcutaneous exposure			
2							
3							

# Column C3: Inhalation Toxicity

0: >20	1: 10-20	2: 2-10 3	: 0.5-2 4:	<0.5 mg/l (4hrs)
Study	rating based on	LC50 value	animal	Details, remarks, please indicate exposure time (hrs)
no.	this study	exp. time	species	
1	4	0,24	Rat	RTECS
2	4	0,18	Mouse	RTECS
3				

Chemical hazard summary sheet	
Tore Syversen	

0: non-irritating 1: Mildly irritating 2: Irritating 3: Severely irritating or corrosive

3A: Corrosi	ve >1 hr-4 hr 3	B: Corrosive >3 min < 1 hr 3C: Corrosive < 3min
study no.	proposed rating	source / kind of study / animal species
1		
2		
3		

#### Column D2: Eye Irritation / Corrosion

0: Not irrit	ating 1: Mild	y irritating 2: Irritating 3: Severely irritating with irreversible corneal injury
study no.	proposed rating	source / kind of study / animal species
1		
2		
3		

## Column D3: Other long term effects (indicate by appropriate letter in box)

Carcinogenic - C	С	Aspiration haz A		Neurotoxic - N	
Lung injury - L		Reprotoxic – R	R	Immunotoxic - I	
Mutagenic - M	Μ	Photosensitizer - P		Sensitizing - S	

# Source/comment:

C: RTECS gives a large range of studies.

R: RTECS gives a range of studies; fetotoxicity, fertility, abnormalities

M: RTECS gives a range of studies; bacteria, yeast, Drosophila, human in vitro

## **Remarks**

# RTECS

RTECS lists a range of toxicology reviews

OccExpLevel: several countries: 0,001 mg/m3 carcinogen

EPA Genotox program. Many positive listings on C and M

EPA IRIS database listed

NIOSH and OSHA analytical methods

NTP 2004: Reasonably anticipated to be a human carcinogen

ACC-2

*Very high acute toxicity Serious long term effects* OEL: 0.001 mg/m3 IRIS: Carcinogen risk from inhalation calculated

C1	C2	C3	D1	D2	D3	Date

Chemical hazard summary sheet	
Tore Syversen	

CAS - No.	Name	
74-89-5	Methylamine	

EU-Risk phrases	
<b>Comments on chemical</b>	
<b>Comments on evaluation</b>	
GESAMP/EHS file	Yes
RTECS file	PF6300000 update:200911
IUCLID file	Yes
REACH file	
Other sources	• CPDB-
	• IRIS-

]	No.	CAS - No.	chemical name	remark
	1			
	2			

# Column C1: Oral Toxicity

0: >200	0: >2000 1: 300-2000 2: 50-300 3: 5-50 4: <5 mg/kg bw						
Study	rating based on	LD50 value	animal	Source or comment			
no.	this study		species				
1	2	100	Rat	RTECS			
2							
3							

# Column C2: Percutaneous Toxicity

0: >200	0: >2000 1: 1000-2000 2: 200-1000 3. 50-200 4: <50 mg/kg bw						
Study	rating based on	LD <sub>50</sub> value	animal	Source or comment			
no.	this study		species				
1							
2							
3							

# **Column C3: Inhalation Toxicity**

0: > 20	1: 10-20	2: 2-10 3	3: 0.5-2 4:	<0.5 mg/l (4hrs)
Study	rating based on	LC50 value	animal	Details, remarks, please indicate exposure time (hrs)
no.	this study	exp. time	species	
1	3	0,97	Rat	2,5 hour exposure. IUCLID
2				
3				

Chemical hazard summary sheet	
Tore Syversen	

0: non-irritating 1: Mildly irritating 2: Irritating 3: Severely irritating or corrosive

3A: Corros	ive $>1$ hr-4 hr $= 3$	3B: Corrosive >3 min < 1 hr	3C: Corrosive < 3min
study no.	proposed rating	source / kind of study / animal s	pecies
1	3	IUCLID	
2			
3			

#### Column D2: Eye Irritation / Corrosion

0: Not irritating 1: Mildly irritating 2: Irritating 3: Severely irritating with irreversible corneal injury

study no.	proposed rating	source / kind of study / animal species
1	2	IUCLID
2		
3		

## Column D3: Other long term effects (indicate by appropriate letter in box)

Carcinogenic - C		Aspiration haz A	Neurotoxic - N	
Lung injury - L		Reprotoxic – R	Immunotoxic - I	
Mutagenic - M	Μ	Photosensitizer - P	Sensitizing - S	
Source/comment:				
M: RTECS				

#### **Remarks**

OEL: 13 mg/m3 (RTECS) ACC2 Moderate acute toxicity. Serious long term effects OEL: 13 mg/m3 (RTECS)

C1	C2	C3	D1	D2	D3	Date
2	(2)	3	?	?	М	

Chemical hazard summary sheet	
Tore Syversen	

CAS - No.	Name
75-04-7	Ethylamine

EU-Risk phrases	
<b>Comments on chemical</b>	
<b>Comments on evaluation</b>	
GESAMP/EHS file	Yes
RTECS file	KH2100000 update: 200911
IUCLID file	Yes
REACH file	
Other sources	• CPDB-
	• IRIS-

No.	CAS - No.	chemical name	remark
1			
2			

#### Column C1: Oral Toxicity

0: >200	00 1: 300-20	00 2: 50-3	00 3: 5-50	4: <5 mg/kg bw
Study no.	rating based on this study	LD <sub>50</sub> value	animal species	Source or comment
1	1	400	Rat	RTECS
2				
3				

# Column C2: Percutaneous Toxicity

0: >200	0: >2000 1: 1000-2000 2: 200-1000 3. 50-200 4: <50 mg/kg bw				
Study	rating based on	LD50 value	animal	Source or comment	
no.	this study		species		
1	2	270	Rabbit	RTECS	
2					
3					

# Column C3: Inhalation Toxicity

0: >20	1: 10-20	2: 2-10 3	: 0.5-2 4:	<0.5 mg/l (4hrs)
Study	rating based on	LC50 value	animal	Details, remarks, please indicate exposure time (hrs)
no.	this study	exp. time	species	
1	1	10	rabbit	RTECS
2				
3				

Chemical hazard summary sheet	
Tore Syversen	

0: non-irritating 1: Mildly irritating 2: Irritating 3: Severely irritating or corrosive

3A: Corrosi	ive $>1$ hr-4 hr 3	3B: Corrosive $>3 \min < 1 hr$	3C: Corrosive < 3min
study no.	proposed rating	source / kind of study / animal sp	ecies
1	1	RTECS	
2			
3			

Column D2: Eye Irritation / Corrosion 0: Not irritating 1: Mildly irritating 2: Irritating 3: Severely irritating with irreversible corneal injury study no I proposed rating I course / hind of study ( ) is a large study of the large study

study no.	proposed rating	source / kind of study / animal species
1	3	IUCLID
2		
3		

### Column D3: Other long term effects (indicate by appropriate letter in box)

Carcinogenic - C	Aspiration haz A	Neurotoxic - N			
Lung injury - L	Reprotoxic – R	Immunotoxic - I			
Mutagenic - M	Photosensitizer - P	Sensitizing - S			
Source/comment:					
IUCLID: Tested for M negative. Not tested for C or R					

# <u>Remarks</u>

OEL: TWA Norway 18 mg/m3 1999 Sweden 18 mg/m3 2005
C1 assign 2 as per GESAMP rating (RTECS gives 1)
ACC
Moderate acute toxicity
IUCLID: Tested for M negative. Not tested for C or R
OEL: 18 mg/m3

#### **GESAMP/EHS Marine transport**

C1	C2	C3	D1	D2	D3	Date
2	2	1				

٦

Chemical hazard summary sheet	
Tore Syversen	

CAS - No.	Name
106-58-1	1,4-dimethyl piperazine

EU-Risk phrases	
<b>Comments on chemical</b>	
<b>Comments on evaluation</b>	
GESAMP/EHS file	No
RTECS file	TL5945000 Update: 199709
IUCLID file	No
REACH file	
Other sources	• CPDB-
	• IRIS-

No.	CAS - No.	chemical name	remark
1			
2			

#### Column C1: Oral Toxicity

0: >200	00 1: 300-20	00 2: 50-3	00 3: 5-50	4: <5 mg/kg bw
Study	rating based on	LD <sub>50</sub> value	animal	Source or comment
no.	this study		species	
1				
2				
3				

# Column C2: Percutaneous Toxicity

0: >200	0: >2000 1: 1000-2000 2: 200-1000 3. 50-200 4: <50 mg/kg bw					
Study	rating based on	LD <sub>50</sub> value	animal	Source or comment		
no.	this study		species			
1	0	2500	mouse			
2						
3						

# Column C3: Inhalation Toxicity

0: >20	1: 10-20	2: 2-10 3	: 0.5-2 4:	<0.5 mg/l (4hrs)
Study	rating based on	LC <sub>50</sub> value	animal	Details, remarks, please indicate exposure time (hrs)
no.	this study	exp. time	species	
1				
2				
3				

Chemical hazard summary sheet	
Tore Syversen	

0: non-irritating 1: Mildly irritating 2: Irritating 3: Severely irritating or corrosive

3A: Corrosi	ive > 1 hr - 4 hr 3	B: Corrosive >3 min < 1 hr 3C: Corrosive < 3min
study no.	proposed rating	source / kind of study / animal species
1		
2		
3		

#### **Column D2: Eye Irritation / Corrosion**

0: Not irrita	ating 1: Mildl	ly irritating 2: Irritating 3: Severely irritating with irreversible corneal injury
study no.	proposed rating	source / kind of study / animal species
1		
2		
3		

# Column D3: Other long term effects (indicate by appropriate letter in box)

Carcinogenic - C	Aspiration haz A	Neurotoxic - N
Lung injury - L	Reprotoxic – R	Immunotoxic - I
Mutagenic - M	Photosensitizer - P	Sensitizing - S
Source/comment:		

# <u>Remarks</u>

RTECS: listed as a drug. See:

Therapie. Volume(issue)/page/year: 9,314,1954

ACC

Very little data

Low dermal acute is not a good indicator here for other acute tox

C1	C2	C3	D1	D2	D3	Date

Chemical hazard summary sheet	
Tore Syversen	

CAS - No.	Name
110-85-0	Piperazine

EU-Risk phrases	
<b>Comments on chemical</b>	
<b>Comments on evaluation</b>	
GESAMP/EHS file	No
RTECS file	TK7800000 Update:200911
IUCLID file	Yes
REACH file	
Other sources	• CPDB-
	• IRIS-

No.	CAS - No.	chemical name	remark
1			
2			

#### Column C1: Oral Toxicity

0: >200	00 1: 300-20	00 2: 50-30	00 3: 5-50	4: <5 mg/kg bw
Study	rating based on	LD50 value	animal	Source or comment
no.	this study		species	
1	1	600	Mouse	RTECS
2	1	1900	Rat	RTECS
3	0	5600	Rat	RTECS-EPA-2003

# Column C2: Percutaneous Toxicity

0: >200	0: >2000 1: 1000-2000 2: 200-1000 3. 50-200 4: <50 mg/kg bw					
Study	rating based on	LD <sub>50</sub> value	animal	Source or comment		
no.	this study		species			
1	0	3700	Rat	RTECS		
2	0	16000	Rat	RTECS-EPA-2003		
3						

# Column C3: Inhalation Toxicity

0: >20	1: 10-20	2: 2-10 3	0.5-2 4:	<0.5 mg/l (4hrs)
Study	rating based on	LC50 value	animal	Details, remarks, please indicate exposure time (hrs)
no.	this study	exp. time	species	
1	2	5,4	Mouse	2 hrs exposure. RTECS-EA-2003
2				
3				

Chemical hazard summary sheet	
Tore Syversen	

0: non-irritating 1: Mildly irritating 2: Irritating 3: Severely irritating or corrosive

	3A: Corrosi	ive >1 hr-4 hr 3	$3B: Corrosive > 3 min < 1 hr \qquad 3C: Corrosive < 3min$				
study no. proposed rating source / kind of study / animal species							
	1	2 Rabbit. RTECS. Borderline to 1					
	2						
	3						

### Column D2: Eye Irritation / Corrosion

0: Not irritating 1: Mildly irritating 2: Irritating 3: Severely irritating with irreversible corneal injury

study no.	proposed rating	source / kind of study / animal species
1	3	Rabbit. RTECS
2		
3		

### **Column D3: Other long term effects (indicate by appropriate letter in box)**

Carcinogenic - C		Aspiration haz A Neurotoxic - N			
Lung injury - L		Reprotoxic – R		Immunotoxic - I	
Mutagenic - M	(M)	Photosensitizer - P		Sensitizing - S	<b>(S)</b>

### Source/comment:

IUCLID: not a S in animals, but positive in humans

IUCLID: not a C on its own, but increased lung adenoma when co-exposure with Na-nitrite IUCLID: not a M

### <u>Remarks</u>

OEL: TWA 0.3 mg/m3 Norway 1999. 0,3 mg/m3 Sweden 2005 IUCLID: confirm data ACC Moderate acute toxicity OEL: 0.3 mg/m3 C-lungadenoma when coexposure with nitrite. In environment with nitrite or nitrates the respective nitrosoamine might be produced. Expect C, M and R as long term serious health effects

C1	C2	C3	D1	D2	D3	Date

Chemical hazard summary sheet	
Tore Syversen	

CAS - No.	Name
111-41-1	N-(2-hydroxyethyl)-ethylenediamine HEED

EU-Risk phrases	
<b>Comments on chemical</b>	
<b>Comments on evaluation</b>	
GESAMP/EHS file	Yes
RTECS file	KJ6300000 Update: 200911
IUCLID file	Yes
<b>REACH file</b>	
Other sources	• CPDB-
	• IRIS-

1	No.	CAS - No.	chemical name	remark
	1			
	2			

### Column C1: Oral Toxicity

0: >200	0: >2000 1: 300-2000 2: 50-300 3: 5-50 4: <5 mg/kg bw						
Study	rating based on	LD <sub>50</sub> value	animal	Source or comment			
no.	this study		species				
1	0	3000	Rat	RTECS			
2	0	3550	Mouse	RTECS			
3							

 Column C2: Percutaneous Toxicity

 0: >2000
 1: 1000-2000
 2: 200-1000
 3. 50-200
 4: <50</td>
 mg/kg bw

Study	rating based on	LD50 value	animal	Source or comment
no.	this study		species	
1	0	2250	Rat	RTECS
2	0	3560	Rabbit	RTECS
3				

### Column C3: Inhalation Toxicity

0: >20	1: 10-20	2: 2-10 3	: 0.5-2 4:	<0.5 mg/l (4hrs)
Study ra	ating based on	LC50 value	animal	Details, remarks, please indicate exposure time (hrs)
no. th	his study	exp. time	species	
1				
2				
3				

Chemical hazard summary sheet	
Tore Syversen	

0: non-irritating 1: Mildly irritating 2: Irritating 3: Severely irritating or corrosive

3A: Corros	ive $>1$ hr-4 hr $\therefore$	3B: Corrosive >3 min < 1 hr	3C: Corrosive < 3min	
study no.	proposed rating	source / kind of study / animal species		
1	1	RTECS		
2	3	IUCLID		
3				

### Column D2: Eye Irritation / Corrosion

0: Not irritating 1: Mildly irritating 2: Irritating 3: Severely irritating with irreversible corneal injury

study no.	proposed rating	source / kind of study / animal species	
1	3	RTECS	
2	2	IUCLID	
3			

### <u>Column D3: Other long term effects (indicate by appropriate letter in box)</u>

Carcinogenic - C		Aspiration haz A		Neurotoxic - N	
Lung injury - L		Reprotoxic – R	R	Immunotoxic - I	
Mutagenic - M	(M)	Photosensitizer - P		Sensitizing - S	S
Source/comment:					
R: RTECS. Developmental. Cardiovascular					
M: RTECS. IUCLID: Ames					

S: IUCLID

### **Remarks**

OEL: 3 mg/m3. Russia 2003

ACC2

Low acute toxicity. Serious long term toxicity

C1	C2	C3	D1	D2	D3	Date
0	0	0			S	

Chemical hazard summary sheet	
Tore Syversen	

CAS - No.	Name
111-42-2	Diethanolamine

EU-Risk phrases	
<b>Comments on chemical</b>	
<b>Comments on evaluation</b>	
GESAMP/EHS file	No
RTECS file	KL2975000 Update: 200911
IUCLID file	No
REACH file	
Other sources	• CPDB-
	• IRIS-

]	No.	CAS - No.	chemical name	remark
	1			
	2			

### Column C1: Oral Toxicity

0: >200	0: >2000 1: 300-2000 2: 50-300 3: 5-50 4: <5 mg/kg bw					
Study	rating based on	LD <sub>50</sub> value	animal	Source or comment		
no.	this study		species			
1	0	2200	Rabbit	RTECS		
2	0	3300	Mouse	RTECS		
3						

 Column C2: Percutaneous Toxicity

 0: >2000
 1: 1000-2000
 2: 200-1000
 3. 50-200
 4: <50</td>
 mg/kg bw

Study no.	rating based on this study	LD <sub>50</sub> value	animal species	Source or comment
1	0	7600	Rabbit	RTECS
2				
3				

### Column C3: Inhalation Toxicity

0: >20 1: 10-20	2: 2-10 3: 0.5-2 4: <	<0.5 mg/l (4hrs)
Study rating based on I	LC <sub>50</sub> value animal	Details, remarks, please indicate exposure time (hrs)
no. this study e	exp. time species	
1 0		IUCLID. Saturated vapor 8 hrs
2		
3		

Chemical hazard summary sheet	
Tore Syversen	

0: non-irritating 1: Mildly irritating 2: Irritating 3: Severely irritating or corrosive

3A: Corros	ive $>1$ hr-4 hr $=3$	3B: Corrosive $>3 \min < 1 hr$	3C: Corrosive < 3min			
study no.	proposed rating	source / kind of study / animal species				
1	1	Rabbit RTECS	Rabbit RTECS			
2						
3						

### Column D2: Eye Irritation / Corrosion

0: Not irritating 1: Mildly irritating 2: Irritating 3: Severely irritating with irreversible corneal injury

study no.	proposed rating	source / kind of study / animal species
1	3	Rabbit RTECS
2		
3		

### <u>Column D3: Other long term effects (indicate by appropriate letter in box)</u>

Carcinogenic - C	С	Aspiration haz A		Neurotoxic - N	
Lung injury - L		Reprotoxic – R	R	Immunotoxic - I	
Mutagenic - M	Μ	Photosensitizer - P		Sensitizing - S	

### Source/comment:

C: RTECS. Liver.

R: RTECS. Maternal. Paternal. Resportion. Abnormalities

M: RTECS

S: IUCLID: not S

IUCLID: See page 194. Probably not a mutagen/carinogen on its own. However, co-exposure with nitrites or nitrosating compounds produce N-nitrosodiethanolamine /CAS 1116-54-7) which is a potent carcinogen

### Remarks

Carcinogen:

IARC: Animal limited. Human inadequate. Group 3. 2000

ACGIH: Confirmed animal. 2009

OEL:

ACGIH TLV-TWA 1 mg/m3. 2009

Norway TWA 15 mg/m3. 1999

Sweden TWA 15 mg/m3. 2005

ACC2

C, M, R: maybe not the compound itself. But will form nitrosoamine (CAS1116-54-7) with nitrites

C1	C2	C3	D1	D2	D3	Date

Chemical hazard summary sheet	
Tore Syversen	

CAS - No.	Name	
124-40-3	Dimethylamine	

EU-Risk phrases	
<b>Comments on chemical</b>	
<b>Comments on evaluation</b>	
GESAMP/EHS file	Yes
RTECS file	IP8750000 update:200911
IUCLID file	Yes
REACH file	
Other sources	• CPDB-
	• IRIS+

No.	CAS - No.	chemical name	remark
1			
2			

### Column C1: Oral Toxicity

0: >200	0: >2000 1: 300-2000 2: 50-300 3: 5-50 4: <5 mg/kg bw					
Study	rating based on	LD <sub>50</sub> value	animal	Source or comment		
no.	this study		species			
1	1	698	Rat	IUCLID		
2	1	316	Rat	IUCLID		
3	2	240	Rabbit	IUCLID		

### Column C2: Percutaneous Toxicity

0: >200	: >2000 1: 1000-2000 2: 200-1000 3. 50-200 4: <50 mg/kg bw					
Study no.	rating based on this study	LD <sub>50</sub> value	animal species	Source or comment		
1	0	3900	Rat	IUCLID		
2						
3						

### Column C3: Inhalation Toxicity

0: >20	1: 10-20	2: 2-10 3	: 0.5-2 4:	<0.5 mg/l (4hrs)
Study	rating based on	LC50 value	animal	Details, remarks, please indicate exposure time (hrs)
no.	this study	exp. time	species	
1		0,07	?	Exposure time not given.RTECS
2	2	3	Rat	2 hours. RTECS. Borderline 3 rating
3	2	8	Mouse	IUCLID

Chemical hazard summary sheet	
Tore Syversen	

0: non-irritating 1: Mildly irritating 2: Irritating 3: Severely irritating or corrosive

3A: Corrosi	ive >1 hr-4 hr	3B: Corrosive $>3 \min < 1 hr$	3C: Corrosive < 3min			
study no.	proposed rating	source / kind of study / animal species				
1	3	IUCLID				
2						
3						

### Column D2: Eye Irritation / Corrosion

0: Not irritating 1: Mildly irritating 2: Irritating 3: Severely irritating with irreversible corneal injury

study no.	proposed rating	source / kind of study / animal species
1	3	IUCLID
2		
3		

### Column D3: Other long term effects (indicate by appropriate letter in box)

Carcinogenic - C	Aspiration haz A	Neurotoxic - N	
Lung injury - L	Reprotoxic – R	Immunotoxic - I	
Mutagenic - M	Photosensitizer - P	Sensitizing - S	S
Source/comment:			
S: IUCLID			

### <u>Remarks</u>

 OEL TWA: Norge 18 mg/m3 1999. Sverige 3,5 mg/m3 2005

 IUCLID: Tested for C, M and R. Many studies – almost all negative

 ACC2

 Moderate acute toxicity

 No indication for C, M or R

 OEL: 3.5 mg/m3

 IRIS file withdrawn

 In presence of nitrous acid may form nitroso-dimethylamine (CAS62-75-9). If such conditions exist then long term serious effects should be anticipated

C1	C2	C3	D1	D2	D3	Date
2	0	2			S	

Chemical hazard summary sheet	
Tore Syversen	

CAS - No.	Name
140-79-4	N,N'-dinitrosopiperazine

EU-Risk phrases	
<b>Comments on chemical</b>	
<b>Comments on evaluation</b>	
<b>GESAMP/EHS file</b>	No
RTECS file	TL6300000 Update 200805
IUCLID file	No
<b>REACH file</b>	
Other sources	• CPDB+
	• IRIS-

No.	CAS - No.	chemical name	remark
1			
2			

### Column C1: Oral Toxicity

0: >200	): >2000 1: 300-2000 2: 50-300 3: 5-50 4: <5 mg/kg bw					
Study	rating based on	LD <sub>50</sub> value	animal	Source or comment		
no.	this study		species			
1	2	160	rat	RTECS		
2						
3						

### Column C2: Percutaneous Toxicity

0: >200	0: >2000 1: 1000-200 2: 200-1000 3. 50-200 4: <50 mg/kg bw					
Study	rating based on	LD50 value	animal	Source or comment		
no.	this study		species			
1	3	160	Rat	RTECS		
2						
3						

### Column C3: Inhalation Toxicity

0: >20	1: 10-20	2: 2-10 3	: 0.5-2 4:	<0.5 mg/l (4hrs)
Study ra	ating based on	LC50 value	animal	Details, remarks, please indicate exposure time (hrs)
no. th	his study	exp. time	species	
1				
2				
3				

Chemical hazard summary sheet	
Tore Syversen	

0: non-irritating 1: Mildly irritating 2: Irritating 3: Severely irritating or corrosive

3A: Corrosi	ve >1 hr-4 hr 3	B: Corrosive >3 min < 1 hr 3C: Corrosive < 3min			
study no.	proposed rating	source / kind of study / animal species			
1					
2					
3					

### Column D2: Eye Irritation / Corrosion

0: Not irritating 1: Mildly irritating 2: Irritating 3: Severely irritating with irreversible corneal injury

study no.	proposed rating	source / kind of study / animal species
1		
2		
3		

### Column D3: Other long term effects (indicate by appropriate letter in box)

Carcinogenic - C	С	Aspiration haz A		Neurotoxic - N	
Lung injury - L		Reprotoxic – R	R	Immunotoxic - I	
Mutagenic - M	Μ	Photosensitizer - P		Sensitizing - S	
Source/commont.					

### Source/comment:

C: RTECS lists a range of studies.

M: RTECS lists several studies

R: RTECS lists three studies

### **Remarks**

EPA Genetox program 1988

Positive: Carcinogenicity-mouse/rat; Cell transform.-mouse embryo

Positive: Host-mediated assay; Histidine reversion-Ames test

Positive: D melanogaster Sex-linked lethal

Inconclusive: D melanogaster-reciprocal translocation

Mutation Research. Volume(issue)/page/year: 635,52,2007

ACC2

High acute toxicity

Expect inhalation hazard

Serious long term effects

C1	C2	C3	D1	D2	D3	Date

Chemical hazard summary sheet	
Tore Syversen	

CAS - No.	Name
142-26-7	N-(2-hydroxyethyl)-acetamide (HEA)

EU-Risk phrases	
<b>Comments on chemical</b>	
<b>Comments on evaluation</b>	
<b>GESAMP/EHS file</b>	No
RTECS file	AC3120000
IUCLID file	No
REACH file	
Other sources	• CPDB-
	• IRIS-

No.	CAS - No.	chemical name	remark
1			
2			

### Column C1: Oral Toxicity

0: >200	0: >2000 1: 300-2000 2: 50-300 3: 5-50 4: <5 mg/kg bw						
Study	rating based on	LD50 value	animal	Source or comment			
no.	this study		species				
1	0	26950	Rat	RTECS			
2							
3							

### Column C2: Percutaneous Toxicity

0: >200	0: >2000 1: 1000-2000 2: 200-1000 3. 50-200 4: <50 mg/kg bw					
Study	rating based on	LD50 value	animal	Source or comment		
no.	this study		species			
1	0	>20000	Rabbit	RTECS		
2						
3						

### Column C3: Inhalation Toxicity

0: >20	1: 10-20	2:2-10	3: 0.5-2 4:	<0.5 mg/l (4hrs)
Study	rating based on	LC50 value	animal	Details, remarks, please indicate exposure time (hrs)
no.	this study	exp. time	species	
1				
2				
3				

Chemical hazard summary sheet	
Tore Syversen	1

0: non-irritating 1: Mildly irritating 2: Irritating 3: Severely irritating or corrosive

	3A: Corrosi	ve >1 hr-4 hr 3	B: Corrosive $>3 \min < 1 hr$ 3C: Corrosive $< 3\min$				
study no. proposed rating source / kind of study / animal species							
	1	1	RTECS rabbit				
	2						
	3						

### **Column D2: Eye Irritation / Corrosion**

0: Not irrit	ating 1: Mildl	y irritating 2: Irritating 3: Severely irritating with irreversible corneal injury			
study no. proposed rating source / kind of study / animal species					
1	<b>3</b> RTECS rabbit				
2					
3					

### Column D3: Other long term effects (indicate by appropriate letter in box)

Carcinogenic - C	Aspiration haz A	Neurotoxic - N					
Lung injury - L	Reprotoxic – R	Immunotoxic - I					
Mutagenic - M Photosensitizer - P Sensitizing - S							
Source/comment:							

## <u>Remarks</u>

Acc2

No comment

C1	C2	C3	D1	D2	D3	Date

Tore Syversen	

CAS - No.	Name			
150-25-4	N,N-Bis(2-hydroxy-ethyl)glycine			

EU-Risk phrases	
Comments on chemical	
<b>Comments on evaluation</b>	
GESAMP/EHS file	No
RTECS file	MB9700000 Update 19901
IUCLID file	No
REACH file	
Other sources	•

<b>Evaluation based on</b> (if b			sed on similar chemical)	
No.	CAS - No.		chemical name	remark
1				
2				

### Column C1: Oral Toxicity

0: >200	00 1: 300-20	00 2: 50-3	00 3: 5-50	4: <5 mg/kg bw
Study	rating based on this study	LD <sub>50</sub> value	animal	Source or comment
no.	uns study		species	
1				
2				
3				

### Column C2: Percutaneous Toxicity

0: >200	0: >2000 1: 1000-2000 2: 200-1000 3. 50-200 4: <50 mg/kg bw						
Study	rating based on	LD <sub>50</sub> value	animal	Source or comment			
no.	this study		species				
1							
2							
3							

### Column C3: Inhalation Toxicity

0: >20	1: 10-20	2: 2-10 3	: 0.5-2 4:	<0.5 mg/l (4hrs)
Study	rating based on	LC50 value	animal	Details, remarks, please indicate exposure time (hrs)
no.	this study	exp. time	species	
1				
2				
3				

Chemical hazard summary sheet	
Tore Syversen	

0: non-irritating 1: Mildly irritating 2: Irritating 3: Severely irritating or corrosive

3A: Corros	ive $>1$ hr-4 hr 3	B: Corrosive $>3 \min < 1 hr$ 3	C: Corrosive < 3min			
study no.	proposed rating	sed rating source / kind of study / animal species				
1						
2						
3						

### Column D2: Eye Irritation / Corrosion

0: Not irrit	ating 1: Mildl	ly irritating 2: Irritating 3: Severely irritating with irreversible corneal injury
study no.	proposed rating	source / kind of study / animal species
1		
2		
3		

### Column D3: Other long term effects (indicate by appropriate letter in box)

Carcinogenic - C	Aspiration haz A	Neurotoxic - N					
Lung injury - L	Reprotoxic – R	Immunotoxic - I					
Mutagenic - M	Photosensitizer - P	Sensitizing - S					
Source/comment:	Source/comment:						

### <u>Remarks</u>

RTECS ip LD50 mouse 1540 mg/kg

ACC2

No relevant data.

*Low ip tox – can assume low acute toxicity.* 

C1	C2	C3	D1	D2	D3	Date

Chemical hazard summary sheet	
Tore Syversen	

CAS - No.	Name
497-25-6	Oxazolidine

EU-Risk phrases	
<b>Comments on chemical</b>	
<b>Comments on evaluation</b>	
GESAMP/EHS file	No
RTECS file	RQ2450000 Update: 199612
IUCLID file	No
REACH file	
Other sources	• CPDB-
	• IRIS-

No.	CAS - No.	chemical name	remark
1			
2			

### Column C1: Oral Toxicity

0: >200	00 1: 300-20	00 2: 50-3	00 3: 5-50	4: <5 mg/kg bw
Study	rating based on	LD <sub>50</sub> value	animal	Source or comment
no.	this study		species	
1				
2				
3				

### Column C2: Percutaneous Toxicity

0: >200	0: >2000 1: 1000-2000 2: 200-1000 3. 50-200 4: <50 mg/kg bw					
Study	rating based on	LD <sub>50</sub> value	animal	Source or comment		
no.	this study		species			
1						
2						
3						

### Column C3: Inhalation Toxicity

0: > 20	1: 10-20	2: 2-10 3	: 0.5-2 4:	<0.5 mg/l (4hrs)
Study	rating based on	LC <sub>50</sub> value	animal	Details, remarks, please indicate exposure time (hrs)
no.	this study	exp. time	species	
1				
2				
3				

Chemical hazard summary sheet	
Tore Syversen	

0: non-irritating 1: Mildly irritating 2: Irritating 3: Severely irritating or corrosive

3A: Corrosi	ive > 1 hr - 4 hr 3	B: Corrosive >3 min < 1 hr 3C: Corrosive < 3min					
study no.	proposed rating	bosed rating source / kind of study / animal species					
1							
2							
3							

### **Column D2: Eye Irritation / Corrosion**

0: Not irrit	0: Not irritating 1: Mildly irritating 2: Irritating 3: Severely irritating with irreversible corneal injury					
study no. proposed rating source / kind of study / animal species						
1						
2						
3						

### Column D3: Other long term effects (indicate by appropriate letter in box)

Carcinogenic - C	(C)	Aspiration haz A		Neurotoxic - N			
Lung injury - L		Reprotoxic – R		Immunotoxic - I			
Mutagenic - M Photosensitizer -				Sensitizing - S			
Source/comment:							
C: RTECS. Skin. Equivocal							

### <u>Remarks</u>

ACC2 RTECS skin cancer equivocal

C1	C2	C3	D1	D2	D3	Date

Chemical hazard summary sheet	
Tore Syversen	

CAS - No.	Name
693-06-1	N-(2-hydroxyethyl)- Formamide (HEF

EU-Risk phrases	
Comments on chemical	
<b>Comments on evaluation</b>	
<b>GESAMP/EHS file</b>	No
RTECS file	No
IUCLID file	No
<b>REACH file</b>	
Other sources	• CDDB-
	• IRIS-

No.	CAS - No.	chemical name	remark
1			
2			

### **Column C1: Oral Toxicity**

0: >200	00 1: 300-20	2: 50-3	00 3: 5-50	4: <5 mg/kg bw
Study	rating based on	LD <sub>50</sub> value	animal	Source or comment
no.	this study		species	
1				
2				
3				

### Column C2: Percutaneous Toxicity

0: >200	00 1: 1000-20	000 2: 200-	1000 3. 50-2	00 4: <50 mg/kg bw
Study	rating based on	LD <sub>50</sub> value	animal	Source or comment
no.	this study		species	
1				
2				
3				

### **Column C3: Inhalation Toxicity**

0: >20	1: 10-20	2: 2-10 3	: 0.5-2 4:	<0.5 mg/l (4hrs)
Study	rating based on	LC50 value	animal	Details, remarks, please indicate exposure time (hrs)
no.	this study	exp. time	species	
1				
2				
3				

\_\_\_\_\_

Chemical hazard summary sheet	
Tore Syversen	

0: non-irritating 1: Mildly irritating 2: Irritating 3: Severely irritating or corrosive

3A: Corrosi	ve >1 hr-4 hr 3	3B: Corrosive $>3 \min < 1$ hr	3C: Corrosive < 3min
study no.	proposed rating	source / kind of study / animal s	species
1			
2			
3			

### Column D2: Eye Irritation / Corrosion

0: Not irrit	ating 1: Mildl	y irritating 2: Irritating 3: Severely irritating with irreversible corneal injury
study no.	proposed rating	source / kind of study / animal species
1		
2		
3		

### <u>Column D3: Other long term effects (indicate by appropriate letter in box)</u>

Carcinogenic - C	Aspiration haz A	Neurotoxic - N				
Lung injury - L	Reprotoxic – R	Immunotoxic - I				
Mutagenic - M	Photosensitizer - P	Sensitizing - S				
Source/comment:						

### Remarks

ACC2			
No data			

C1	C2	C3	D1	D2	D3	Date

Chemical hazard summary sheet	
Tore Syversen	

CAS - No.	Name
924-16-3	n-butyl-n-nitroso-1-butanamine

EU-Risk phrases	
<b>Comments on chemical</b>	
<b>Comments on evaluation</b>	
GESAMP/EHS file	No
RTECS file	EJ4025000 Update: 200908
IUCLID file	
REACH file	
Other sources	•

No.	CAS - No.	chemical name	remark
1			
2			

### Column C1: Oral Toxicity

0: >200	00 1: 300-20	2: 50-3	00 3: 5-50	4: <5 mg/kg bw
Study	rating based on	LD <sub>50</sub> value	animal	Source or comment
no.	this study		species	
1	1	1200	Rat	RTECS
2	0	2150	Hamster	RTECS
3				

### Column C2: Percutaneous Toxicity

0: >200	0: >2000 1: 1000-2000 2: 200-1000 3. 50-200 4: <50 mg/kg bw					
Study	rating based on	LD50 value	animal	Source or comment		
no.	this study		species			
1	1	1200	Rat	RTECS		
2	2	561	Hamster	RTECS		
3						

### Column C3: Inhalation Toxicity

0: >20	1: 10-20	2: 2-10 3	: 0.5-2 4:	<0.5 mg/l (4hrs)
Study no.	rating based on this study	$LC_{50}$ value exp. time	animal species	Details, remarks, please indicate exposure time (hrs)
1				
2				
3				

Chemical hazard summary sheet	
Tore Syversen	

0: non-irritating 1: Mildly irritating 2: Irritating 3: Severely irritating or corrosive

3A: Corros	ive $>1$ hr-4 hr 3	BB: Corrosive $>3 \min < 1 hr$	3C: Corrosive < 3min
study no.	proposed rating	source / kind of study / animal s	pecies
1			
2			
3			

### **Column D2: Eye Irritation / Corrosion**

0: Not irrita	ating 1: Mildl	y irritating 2: Irritating 3: Severely irritating with irreversible corneal injury
study no.	proposed rating	source / kind of study / animal species
1		
2		
3		

### Column D3: Other long term effects (indicate by appropriate letter in box)

Carcinogenic - C	С	Aspiration haz A		Neurotoxic - N				
Lung injury - L		Reprotoxic – R	R	Immunotoxic - I				
Mutagenic - M	Μ	Photosensitizer - P		Sensitizing - S				
Source/comment:								
C: RTECS many studies; kidney, liver, GI, respiratory								

R: RTECS several studies mainly fetotoxicity

M: RTECS many studies

### <u>Remarks</u>

IARC: animal sufficient, human no adequate data. Group 2B classified in 1987 OEL: Austria and Switzerland: 0.001-0.0025 mg/m3 (2006) NTP: reasonably anticipated to be a human carcinogen (2004)

C1	C2	C3	D1	D2	D3	Date

Chemical hazard summary sheet	
Tore Syversen	

CAS - No.	Name
1116-54-7	N-nitrosodiethanolamine

EU-Risk phrases	
<b>Comments on chemical</b>	
<b>Comments on evaluation</b>	
GESAMP/EHS file	No
RTECS file	KL9550000 Update: 200905
IUCLID file	No
REACH file	
Other sources	• CPDB+
	• IRIS+

No.	CAS - No.	chemical name	remark
1			
2			

### Column C1: Oral Toxicity

0: >200	00 1: 300-20	00 2: 50-3	00 3: 5-50	4: <5 mg/kg bw
Study	rating based on	LD <sub>50</sub> value	animal	Source or comment
no.	this study		species	
1	0	7500	Rat	RTECS
2				
3				

### Column C2: Percutaneous Toxicity

0:	>200	00	1:	1000-2	000	2: 200-	1000	3.	50-200	4: <50	mg/kg bw	
				-								

Study	rating based on	LD <sub>50</sub> value	animal	Source or comment
no.	this study		species	
1	(0)	-	Hamster	LDLo=11000 mg/kg – RTECS. Subcutaneous
2				
3				

### Column C3: Inhalation Toxicity

0: >20	1: 10-20	2: 2-10 3:	: 0.5-2 4:	<0.5 mg/l (4hrs)
Study	rating based on	LC50 value	animal	Details, remarks, please indicate exposure time (hrs)
no.	this study	exp. time	species	
1				
2				
3				

Chemical hazard summary sheet	
Tore Syversen	

0: non-irritating 1: Mildly irritating 2: Irritating 3: Severely irritating or corrosive

3A: Corros	ive >1 hr-4 hr $3$	BB: Corrosive $>3 \min < 1 hr$	3C: Corrosive < 3min
study no.	proposed rating	source / kind of study / animal s	pecies
1			
2			
3			

### **Column D2: Eye Irritation / Corrosion**

0: Not irrit	ating 1: Mildl	ly irritating 2: Irritating 3: Severely irritating with irreversible corneal injury
study no.	proposed rating	source / kind of study / animal species
1		
2		
3		

### Column D3: Other long term effects (indicate by appropriate letter in box)

Carcinogenic - C	С	Aspiration haz A		Neurotoxic - N				
Lung injury - L Reprotoxic – R (R) Immunotoxic				Immunotoxic - I				
Mutagenic - M								
Source/comment:								
C: RTECS many studies; liver, respiratory								
M: RTECS many studies								
(R): By compare with other nitroso compounds								

### <u>Remarks</u>

IARC: Animal sufficient, human inadequate. Group 2B. Classified 2000			
OEL: Austria and Switzerland: 0.001-0.0025 mg/m3 (2006)			
ACC2			
Non-toxic by oral or dermal route.			
No data on reproductive effects			
Serious long term effects			
OEL: 0.001 mg/m3			
IRIS on oral intake			

C1	C2	C3	D1	D2	D3	Date

Chemical hazard summary sheet	
Tore Syversen	

CAS - No.	Name
1615-14-1	N-(2-hydroxy-ethyl)imidazole (HEI)

EU-Risk phrases	
<b>Comments on chemical</b>	
<b>Comments on evaluation</b>	
<b>GESAMP/EHS file</b>	No
RTECS file	No
IUCLID file	No
REACH file	
Other sources	• CPDB-
	• IRIS-

No.	CAS - No.	chemical name	remark
1			
2			

#### Column C1: Oral Toxicity

0: >200	00 1: 300-20	00 2: 50-3	00 3: 5-50	4: <5 mg/kg bw
Study	rating based on	LD <sub>50</sub> value	animal	Source or comment
no.	this study		species	
1				
2				
3				

### Column C2: Percutaneous Toxicity

0: >200	00 1: 1000-20	000 2: 200-	1000 3. 50-2	00 4: <50 mg/kg bw
Study	rating based on	LD <sub>50</sub> value	animal	Source or comment
no.	this study		species	
1				
2				
3				

### Column C3: Inhalation Toxicity

0: >20	1: 10-20	2: 2-10 3	: 0.5-2 4:	<0.5 mg/l (4hrs)
Study	rating based on	LC <sub>50</sub> value	animal	Details, remarks, please indicate exposure time (hrs)
no.	this study	exp. time	species	
1				
2				
3				

Chemical hazard summary sheet	
Tore Syversen	

0: non-irritating 1: Mildly irritating 2: Irritating 3: Severely irritating or corrosive

3A: Corrosi	ive > 1 hr - 4 hr 3	B: Corrosive >3 min < 1 hr 3C: Corrosive < 3min
study no.	proposed rating	source / kind of study / animal species
1		
2		
3		

### **Column D2: Eye Irritation / Corrosion**

0: Not irritating 1: Mildly		y irritating 2: Irritating 3: Severely irritating with irreversible corneal injury
study no.	proposed rating	source / kind of study / animal species
1		
2		
3		

### Column D3: Other long term effects (indicate by appropriate letter in box)

Carcinogenic - C	Aspiration haz A	Neurotoxic - N				
Lung injury - L	Reprotoxic – R	Immunotoxic - I				
Mutagenic - M	Photosensitizer - P	Sensitizing - S				
Source/comment:						

# <u>Remarks</u>

ACC2

No data

C1	C2	C3	D1	D2	D3	Date

Chemical hazard summary sheet	
Tore Syversen	

CAS - No.	Name
3699-54-5	1-(2 hydroxyethyl)-2-imidazolidinone (HEIA

EU-Risk phrases	
<b>Comments on chemical</b>	
<b>Comments on evaluation</b>	
GESAMP/EHS file	No
RTECS file	No
IUCLID file	No
REACH file	
Other sources	• PDB-
	• IRIS-

No.	CAS - No.	chemical name	remark
1			
2			

#### Column C1: Oral Toxicity

0: >200	00 1: 300-20	00 2: 50-3	00 3: 5-50	4: <5 mg/kg bw
Study	rating based on	LD <sub>50</sub> value	animal	Source or comment
no.	this study		species	
1				
2				
3				

### Column C2: Percutaneous Toxicity

0: >200	00 1: 1000-20	000 2: 200-	1000 3. 50-2	00 4: <50 mg/kg bw
Study	rating based on	LD <sub>50</sub> value	animal	Source or comment
no.	this study		species	
1				
2				
3				

### Column C3: Inhalation Toxicity

0: >20	1: 10-20	2: 2-10 3	: 0.5-2 4:	<0.5 mg/l (4hrs)
Study	rating based on	LC <sub>50</sub> value	animal	Details, remarks, please indicate exposure time (hrs)
no.	this study	exp. time	species	
1				
2				
3				

Chemical hazard summary sheet	
Tore Syversen	

0: non-irritating 1: Mildly irritating 2: Irritating 3: Severely irritating or corrosive

3A: Corros	ive $>1$ hr-4 hr 3	B: Corrosive >3 min < 1 hr	3C: Corrosive < 3min
study no.	proposed rating	source / kind of study / animal spo	ecies
1			
2			
3			

### **Column D2: Eye Irritation / Corrosion**

0: Not irritating 1: Mildl		ly irritating 2: Irritating 3: Severely irritating with irreversible corneal injury
study no.	proposed rating	source / kind of study / animal species
1		
2		
3		

### Column D3: Other long term effects (indicate by appropriate letter in box)

Carcinogenic - C	Aspiration haz A	Neurotoxic - N				
Lung injury - L	Reprotoxic – R	Immunotoxic - I				
Mutagenic - M	Photosensitizer - P	Sensitizing - S				
Source/comment:						

# <u>Remarks</u>

ACC2

No data

C1	C2	C3	D1	D2	D3	Date

Chemical hazard summary sheet	
Tore Syversen	

CAS - No.	Name
4164-28-7	Dimethylnitramine

EU-Risk phrases	
<b>Comments on chemical</b>	
<b>Comments on evaluation</b>	
GESAMP/EHS file	No
RTECS file	IQ450000 Update: 200711
IUCLID file	No
REACH file	
Other sources	• CPDB+
	• IRIS-

No.	CAS - No.	chemical name	remark
1			
2			

### Column C1: Oral Toxicity

0: >200	00 1: 300-20	00 2: 50-3	00 3: 5-50	4: <5 mg/kg bw
Study	rating based on	LD50 value	animal	Source or comment
no.	this study		species	
1	1	1095		RTECS
2				
3				

### Column C2: Percutaneous Toxicity

0: >200	00 1: 1000-20	000 2: 200-	1000 3. 50-2	00 4: <50 mg/kg bw
Study	rating based on	LD <sub>50</sub> value	animal	Source or comment
no.	this study		species	
1				
2				
3				

### Column C3: Inhalation Toxicity

0: >20	1: 10-20	2: 2-10 3	: 0.5-2 4:	<0.5 mg/l (4hrs)
Study	rating based on	LC <sub>50</sub> value	animal	Details, remarks, please indicate exposure time (hrs)
no.	this study	exp. time	species	
1				
2				
3				

Chemical hazard summary sheet	
Tore Syversen	

0: non-irritating 1: Mildly irritating 2: Irritating 3: Severely irritating or corrosive

3A: Corrosi	ive > 1 hr - 4 hr 3	B: Corrosive >3 min < 1 hr 3C: Corrosive < 3min
study no.	proposed rating	source / kind of study / animal species
1		
2		
3		

### **Column D2: Eye Irritation / Corrosion**

0: Not irritating 1: Mildly		ly irritating 2: Irritating 3: Severely irritating with irreversible corneal injury
study no.	proposed rating	source / kind of study / animal species
1		
2		
3		

### Column D3: Other long term effects (indicate by appropriate letter in box)

Carcinogenic - C	С	Aspiration haz A		Neurotoxic - N			
Lung injury - L		Reprotoxic – R		Immunotoxic - I			
Mutagenic - M		Photosensitizer - P		Sensitizing - S			
Source/comment:							
C: Equivocal data from RTECS							
C: CPDB	1						

### <u>Remarks</u>

ACC2 Equivocal RTECS C based on CPDB *Serious long term effects* 

C1	C2	C3	D1	D2	D3	Date

Chemical hazard summary sheet	
Tore Syversen	

CAS - No.	Name
4164-37-8	N,N'-dinitropiperazine

EU-Risk phrases	
<b>Comments on chemical</b>	
<b>Comments on evaluation</b>	
GESAMP/EHS file	No
RTECS file	TL6290000 update:199712
IUCLID file	No
REACH file	
Other sources	• CPDB-
	• IRIS-

No.	CAS - No.	chemical name	remark
1			
2			

### Column C1: Oral Toxicity

0: >200	00 1: 300-20	00 2: 50-3	00 3: 5-50	4: <5 mg/kg bw
Study	rating based on	LD <sub>50</sub> value	animal	Source or comment
no.	this study		species	
1				
2				
3				

### Column C2: Percutaneous Toxicity

0: >200	0: >2000 1: 1000-2000 2: 200-1000 3. 50-200 4: <50 mg/kg bw						
Study	rating based on	LD <sub>50</sub> value	animal	Source or comment			
no.	this study		species				
1							
2							
3							

### Column C3: Inhalation Toxicity

0: >20	1: 10-20	2: 2-10 3	: 0.5-2 4:	<0.5 mg/l (4hrs)
Study	rating based on	LC <sub>50</sub> value	animal	Details, remarks, please indicate exposure time (hrs)
no.	this study	exp. time	species	
1				
2				
3				

Chemical hazard summary sheet	
Tore Syversen	

0: non-irritating 1: Mildly irritating 2: Irritating 3: Severely irritating or corrosive

3A: Corrosi	ive > 1 hr - 4 hr 3	B: Corrosive >3 min < 1 hr 3C: Corrosive < 3min
study no.	proposed rating	source / kind of study / animal species
1		
2		
3		

### **Column D2: Eye Irritation / Corrosion**

0: Not irrita	ating 1: Mildl	y irritating 2: Irritating 3: Severely irritating with irreversible corneal injury
study no.	proposed rating	source / kind of study / animal species
1		
2		
3		

### Column D3: Other long term effects (indicate by appropriate letter in box)

Carcinogenic - C	Aspiration haz A	Neurotoxic - N				
Lung injury - L	Reprotoxic – R	Immunotoxic - I				
Mutagenic - M	Photosensitizer - P	Sensitizing - S				
Source/comment:	Source/comment:					

### <u>Remarks</u>

 RTECS: One entry on LD50 ip mouse 48 mg/kg

 ACC2

 No relevant data

 Two O-N=O groups. Could be reactive and a potential C

C1	C2	C3	D1	D2	D3	Date

Chemical hazard summary sheet	
Tore Syversen	

CAS - No.	Name
5464-12-0	4-methyl-1-Piperazineethanol

EU-Risk phrases	
<b>Comments on chemical</b>	
<b>Comments on evaluation</b>	
<b>GESAMP/EHS file</b>	No
RTECS file	No
IUCLID file	No
<b>REACH file</b>	
Other sources	• CPDB-
	• IRIS-

No.	CAS - No.	chemical name	remark
1			
2			

### Column C1: Oral Toxicity

0: >200	00 1: 300-20	2: 50-3	00 3: 5-50	4: <5 mg/kg bw
Study	rating based on	LD <sub>50</sub> value	animal	Source or comment
no.	this study		species	
1				
2				
3				

### Column C2: Percutaneous Toxicity

0: > 20	00 1: 1000-2	000 2: 200-	1000 3. 50-2	00 4: <50 mg/kg bw
Study	rating based on	LD <sub>50</sub> value	animal	Source or comment
no.	this study		species	
1				
2				

### **Column C3: Inhalation Toxicity**

3

0: >20	1: 10-20	2: 2-10 3	: 0.5-2 4:	<0.5 mg/l (4hrs)
Study	rating based on	LC50 value	animal	Details, remarks, please indicate exposure time (hrs)
no.	this study	exp. time	species	
1				
2				
3				

Chemical hazard summary sheet	
Tore Syversen	

0: non-irritating 1: Mildly irritating 2: Irritating 3: Severely irritating or corrosive

3A: Corrosi	1  ve > 1  hr - 4  hr = 3	B: Corrosive $>3$ min $< 1$ hr	3C: Corrosive < 3min
study no.	proposed rating	source / kind of study / animal sp	ecies
1			
2			
3			

### Column D2: Eye Irritation / Corrosion

0: Not irrit	ating 1: Mildl	y irritating 2: Irritating 3: Severely irritating with irreversible corneal injury
study no.	proposed rating	source / kind of study / animal species
1		
2		
3		

### Column D3: Other long term effects (indicate by appropriate letter in box)

Carcinogenic - C	Aspiration haz A	Neurotoxic - N				
Lung injury - L	Reprotoxic – R	Immunotoxic - I				
Mutagenic - M	Photosensitizer - P	Sensitizing - S				
Source/comment:	Source/comment:					

### **Remarks**

ACC No data

C1	C2	C3	D1	D2	D3	Date

Chemical hazard summary sheet	
Tore Syversen	

CAS - No.	Name	
5632-47-3	1-Nitrosopiperazine	

EU-Risk phrases	
<b>Comments on chemical</b>	
<b>Comments on evaluation</b>	
GESAMP/EHS file	No
RTECS file	TM2450000 Update: 200905
IUCLID file	No
REACH file	
Other sources	• CPDB+
	• IRIS-

No.	CAS - No.	chemical name	remark
1			
2			

#### Column C1: Oral Toxicity

0: >200	00 1: 300-20	00 2: 50-30	00 3: 5-50	4: <5 mg/kg bw
Study	rating based on	LD <sub>50</sub> value	animal	Source or comment
no.	this study		species	
1	0	2260	Rat	RTECS
2				
3				

### Column C2: Percutaneous Toxicity

0: >200	00 1: 1000-20	00 2: 200-1	000 3. 50-20	0 4: <50 mg/kg bw
Study no.	rating based on this study	LD <sub>50</sub> value	animal species	Source or comment
1				
2				
3				

### Column C3: Inhalation Toxicity

0: >20	1: 10-20	2: 2-10 3	: 0.5-2 4:	<0.5 mg/l (4hrs)
Study	rating based on	LC <sub>50</sub> value	animal	Details, remarks, please indicate exposure time (hrs)
no.	this study	exp. time	species	
1				
2				
3				

Chemical hazard summary sheet	
Tore Syversen	

0: non-irritating 1: Mildly irritating 2: Irritating 3: Severely irritating or corrosive

3A: Corros	sive $>1$ hr-4 hr $=3$	3B: Corrosive >3 min < 1 hr	3C: Corrosive < 3min
study no.	proposed rating	source / kind of study / animal s	pecies
1			
2			
3			

### **Column D2: Eye Irritation / Corrosion**

0: Not irritating 1: Mildl		y irritating 2: Irritating 3: Severely irritating with irreversible corneal injury
study no.	proposed rating	source / kind of study / animal species
1		
2		
3		

### Column D3: Other long term effects (indicate by appropriate letter in box)

Carcinogenic - C	С	Aspiration haz A		Neurotoxic - N	
Lung injury - L		Reprotoxic – R		Immunotoxic - I	
Mutagenic - M	Μ	Photosensitizer - P		Sensitizing - S	
Sauracleomment					

### Source/comment:

C: RTECS Three studies exposure for 20-60 weeks intermittent. Studies from 1970 and 1975 M: RTECS Three studies

### <u>Remarks</u>

EPA Genetox Program 1988:

Positiv in host-mediated assay

Inconclusiv in histidine reversion-Ames test

Toxicology and Applied Pharmacology. Volume(issue)/page/year: 231,197,2008

ACC2:

*Remarkable low oral toxicity – <u>questionable</u>!* 

No data on reproductive effects, but such effects is to be expected.

Serious long term effects

C1	C2	C3	D1	D2	D3	Date

Chemical hazard summary sheet	
Tore Syversen	

CAS - No.	Name
15833-17-7	3,4,4-trimethyl oxazolidin-2-one

EU-Risk phrases	
<b>Comments on chemical</b>	
<b>Comments on evaluation</b>	
<b>GESAMP/EHS file</b>	No
RTECS file	No
IUCLID file	No
<b>REACH file</b>	
Other sources	• CPDB-
	• IRIS-

No.	CAS - No.	chemical name	remark
1			
2			

### Column C1: Oral Toxicity

0: >200	00 1: 300-20	2: 50-3	00 3: 5-50	4: <5 mg/kg bw
Study	rating based on	LD <sub>50</sub> value	animal	Source or comment
no.	this study		species	
1				
2				
3				

### Column C2: Percutaneous Toxicity

0: >200	00 1: 1000-20	2: 200-	1000 3. 50-2	00 4: <50 mg/kg bw
Study	rating based on	LD <sub>50</sub> value	animal	Source or comment
no.	this study		species	
1				
2				

### **Column C3: Inhalation Toxicity**

3

0: >20	1: 10-20	2: 2-10 3	: 0.5-2 4:	<0.5 mg/l (4hrs)
Study	rating based on	LC50 value	animal	Details, remarks, please indicate exposure time (hrs)
no.	this study	exp. time	species	
1				
2				
3				

Chemical hazard summary sheet	
Tore Syversen	

0: non-irritating 1: Mildly irritating 2: Irritating 3: Severely irritating or corrosive

3A: Corrosi	1  ve > 1  hr - 4  hr = 3	B: Corrosive $>3$ min $< 1$ hr	3C: Corrosive < 3min
study no.	proposed rating	source / kind of study / animal sp	ecies
1			
2			
3			

### Column D2: Eye Irritation / Corrosion

0: Not irrit	ating 1: Mildl	y irritating 2: Irritating 3: Severely irritating with irreversible corneal injury
study no.	proposed rating	source / kind of study / animal species
1		
2		
3		

### <u>Column D3: Other long term effects (indicate by appropriate letter in box)</u>

Carcinogenic - C	Aspiration haz A	Neurotoxic - N				
Lung injury - L	Reprotoxic – R	Immunotoxic - I				
Mutagenic - M	Photosensitizer - P	Sensitizing - S				
Source/comment:						

### Remarks

ACC2			
No data			

C1	C2	C3	D1	D2	D3	Date

Chemical hazard summary sheet	
Tore Syversen	

CAS - No.	Name	
23936-04-1	4-(2-hydroxyethyl)-2-Piperazinone	

EU-Risk phrases	
<b>Comments on chemical</b>	
<b>Comments on evaluation</b>	
GESAMP/EHS file	No
RTECS file	No
IUCLID file	No
REACH file	
Other sources	• CPDB-
	• IRIS-

No.	CAS - No.	chemical name	remark
1			
2			

### Column C1: Oral Toxicity

0: >200	00 1: 300-20	2: 50-3	00 3: 5-50	4: <5 mg/kg bw
Study no.	rating based on this study	LD <sub>50</sub> value	animal species	Source or comment
1				
2				
3				

### Column C2: Percutaneous Toxicity

0: >200	0: >2000 1: 1000-2000 2: 200-1000 3. 50-200 4: <50 mg/kg bw					
Study	rating based on	LD <sub>50</sub> value	animal	Source or comment		
no.	this study		species			
1						
2						
3						

 
 Column C3: Inhalation Toxicity

 0: >20
 1: 10-20
 2: 2-10
 3: 0.5-2
 4: <0.5</td>
 mg/l (4hrs)

Study no.	rating based on this study	$LC_{50}$ value exp. time	animal species	Details, remarks, please indicate exposure time (hrs)
1				
2				
3				

Chemical hazard summary sheet	
Tore Syversen	

0: non-irritating 1: Mildly irritating 2: Irritating 3: Severely irritating or corrosive

3A: Corro	sive $>1$ hr-4 hr 3	3B: Corrosive $>3 \min < 1 hr$	3C: Corrosive < 3min
study no.	proposed rating	source / kind of study / animal s	pecies
1			
2			
3			

### **Column D2: Eye Irritation / Corrosion**

0: Not irrit	ating 1: Mildl	y irritating 2: Irritating 3: Severely irritating with irreversible corneal injury
study no.	proposed rating	source / kind of study / animal species
1		
2		
3		

### Column D3: Other long term effects (indicate by appropriate letter in box)

Carcinogenic - C	Aspiration haz A	Neurotoxic - N				
Lung injury - L	Reprotoxic – R	Immunotoxic - I				
Mutagenic - M	Photosensitizer - P	Sensitizing - S				
Source/comment:						

## <u>Remarks</u>

ACC2

No data

C1	C2	C3	D1	D2	D3	Date

Chemical hazard summary sheet	
Tore Syversen	

CAS - No.	Name
26654-39-7	4,4-dimethyl-2-Oxazolidinone

EU-Risk phrases	
<b>Comments on chemical</b>	
<b>Comments on evaluation</b>	
GESAMP/EHS file	No
RTECS file	No
IUCLID file	No
REACH file	
Other sources	• CPDB-
	• IRIS-

No.	CAS - No.	chemical name	remark
1			
2			

### Column C1: Oral Toxicity

0: >200	0: >2000 1: 300-2000 2: 50-300 3: 5-50 4: <5 mg/kg bw					
Study	rating based on	LD <sub>50</sub> value	animal	Source or comment		
no.	this study		species			
1						
2						
3						

### Column C2: Percutaneous Toxicity

0: >200	0: >2000 1: 1000-2000 2: 200-1000 3. 50-200 4: <50 mg/kg bw					
Study	rating based on	LD <sub>50</sub> value	animal	Source or comment		
no.	this study		species			
1						
2						
3						

### Column C3: Inhalation Toxicity

0: >20	1: 10-20	2: 2-10 3	: 0.5-2 4:	<0.5 mg/l (4hrs)
Study	rating based on	LC <sub>50</sub> value	animal	Details, remarks, please indicate exposure time (hrs)
no.	this study	exp. time	species	
1				
2				
3				

Chemical hazard summary sheet	
Tore Syversen	

0: non-irritating 1: Mildly irritating 2: Irritating 3: Severely irritating or corrosive

3A: Corro	sive $>1$ hr-4 hr $=3$	3B: Corrosive $>3 \min < 1 hr$	3C: Corrosive < 3min	
study no.	proposed rating	source / kind of study / animal s	species	
1				
2				
3				

### **Column D2: Eye Irritation / Corrosion**

0: Not irrita	ating 1: Mildl	ly irritating 2: Irritating 3: Severely irritating with irreversible corneal injury
study no.	proposed rating	source / kind of study / animal species
1		
2		
3		

### Column D3: Other long term effects (indicate by appropriate letter in box)

Carcinogenic - C	Aspiration haz A	Neurotoxic - N					
Lung injury - L	Reprotoxic – R	Immunotoxic - I					
Mutagenic - M	Photosensitizer - P	Sensitizing - S					
Source/comment:	Source/comment:						

## <u>Remarks</u>

ACC2

No data

C1	C2	C3	D1	D2	D3	Date

Chemical hazard summary sheet	
Tore Syversen	

CAS - No.	Name
26921-68-6	2-(methylnitrosoamino)-ethanol

EU-Risk phrases	
<b>Comments on chemical</b>	
<b>Comments on evaluation</b>	
<b>GESAMP/EHS file</b>	No
RTECS file	KL7631000 Update: 200802
IUCLID file	No
REACH file	
Other sources	• CPDB+
	• IRIS-

No.	CAS - No.	chemical name	remark
1			
2			

#### Column C1: Oral Toxicity

0: >200	00 1: 300-20	2: 50-3	00 3: 5-50	4: <5 mg/kg bw
Study no.	rating based on this study	LD <sub>50</sub> value	animal species	Source or comment
1			species	
2				
3				

### Column C2: Percutaneous Toxicity

0: >200	00 1: 1000-20	00 2: 200-1	000 3. 50-20	0 4: <50 mg/kg bw
Study no.	rating based on this study	LD <sub>50</sub> value	animal species	Source or comment
1				
2				
3				

### Column C3: Inhalation Toxicity

0: >20	1: 10-20	2: 2-10 3	: 0.5-2 4:	<0.5 mg/l (4hrs)
Study	rating based on	LC <sub>50</sub> value	animal	Details, remarks, please indicate exposure time (hrs)
no.	this study	exp. time	species	
1				
2				
3				

Chemical hazard summary sheet	
Tore Syversen	

0: non-irritating 1: Mildly irritating 2: Irritating 3: Severely irritating or corrosive

3A: Corros	ive >1 hr-4 hr $3$	BB: Corrosive $>3 \min < 1 hr$	3C: Corrosive < 3min
study no.	proposed rating	source / kind of study / animal s	species
1			
2			
3			

### **Column D2: Eye Irritation / Corrosion**

0: Not irrita	ating 1: Mildl	y irritating 2: Irritating 3: Severely irritating with irreversible corneal injury
study no.	proposed rating	source / kind of study / animal species
1		
2		
3		

### Column D3: Other long term effects (indicate by appropriate letter in box)

Carcinogenic - C	С	Aspiration haz A		Neurotoxic - N		
Lung injury - L		Reprotoxic – R	(R)	Immunotoxic - I		
Mutagenic - M	Μ	Photosensitizer - P		Sensitizing - S		
Source/comment:						
C: RTECS. Oral rat. Liver. 1988						
M: RTECS. DNA d	lamage af	ter oral rat. DNA adduct	after ip m	louse		

R: Nitroso by compare

### <u>Remarks</u>

Review: Mutation Research. (Elsevier Science Pub. B.V., POB 211, 1000 AE Amsterdam, Netherlands) V.1- 1964- Volume(issue)/page/year: 584,1,2005

ACC2

No data on acute effects No data on reproductive effects *Serious long term effects* 

C1	C2	C3	D1	D2	D3	Date

Chemical hazard summary sheet	
Tore Syversen	

CAS - No.	Name
27646-80-6	2-methyl-2-(methylamino)- 1-Propanol

<b>EU-Risk phrases</b>	
<b>Comments on chemical</b>	
Comments on evaluation	
GESAMP/EHS file	No
RTECS file	No
IUCLID file	No
REACH file	
Other sources	•

No.	CAS - No.	chemical name	remark
1			
2			

#### Column C1: Oral Toxicity

0: >200	00 1: 300-20	00 2: 50-3	00 3: 5-50	4: <5 mg/kg bw
Study no.	rating based on this study	LD <sub>50</sub> value	animal species	Source or comment
1				
2				
3				

 Column C2: Percutaneous Toxicity

 0: >2000
 1: 1000-2000
 2: 200-1000
 3. 50-200
 4: <50</td>
 mg/kg bw

Study no.	rating based on this study	LD <sub>50</sub> value	animal species	Source or comment
1				
2				
3				

### Column C3: Inhalation Toxicity

0: >20	1: 10-20	2: 2-10 3	: 0.5-2 4:	<0.5 mg/l (4hrs)
Study	rating based on	LC <sub>50</sub> value	animal	Details, remarks, please indicate exposure time (hrs)
no.	this study	exp. time	species	
1				
2				
3				

Chemical hazard summary sheet	
Tore Syversen	

0: non-irritating 1: Mildly irritating 2: Irritating 3: Severely irritating or corrosive

3A: Corrosive $\geq 1$ hr-4 hr 3B: Corrosive $\geq 3$ min $\leq 1$ hr 3C: Corrosive $\leq 3$ min					
study no.	proposed rating	source / kind of study / animal species			
1					
2					
3					

### **Column D2: Eye Irritation / Corrosion**

0: Not irrita	ating 1: Mildl	y irritating 2: Irritating 3: Severely irritating with irreversible corneal injury
study no.	proposed rating	source / kind of study / animal species
1		
2		
3		

### Column D3: Other long term effects (indicate by appropriate letter in box)

Carcinogenic - C	Aspiration haz A	Neurotoxic - N					
Lung injury - L	Reprotoxic – R	Immunotoxic - I					
Mutagenic - M	Photosensitizer - P	Sensitizing - S					
Source/comment:	Source/comment:						

### <u>Remarks</u>

ACC

No data

C1	C2	C3	D1	D2	D3	Date

Chemical hazard summary sheet	
Tore Syversen	

CAS - No.	Name
42499-41-2	1-nitro-piperazine

EU-Risk phrases	
<b>Comments on chemical</b>	
<b>Comments on evaluation</b>	
GESAMP/EHS file	No
RTECS file	No
IUCLID file	No
REACH file	
Other sources	• CPDB-
	• IRIS-

No.	CAS - No.	chemical name	remark
1			
2			

### Column C1: Oral Toxicity

0: >200	00 1: 300-20	2: 50-3	00 3: 5-50	4: <5 mg/kg bw
Study no.	rating based on this study	LD <sub>50</sub> value	animal species	Source or comment
1				
2				
3				

### Column C2: Percutaneous Toxicity

0: >200	0: >2000 1: 1000-2000 2: 200-1000 3. 50-200 4: <50 mg/kg bw							
Study	rating based on	LD50 value	animal	Source or comment				
no.	this study		species					
1								
2								
3								

### Column C3: Inhalation Toxicity

0: >20 1: 10-20 2: 2-10 3: 0.5-2 4: <0.5 mg/l (4hrs)

Study no.	rating based on this study	$LC_{50}$ value exp. time	animal species	Details, remarks, please indicate exposure time (hrs)
1				
2				
3				

Chemical hazard summary sheet	
Tore Syversen	

0: non-irritating 1: Mildly irritating 2: Irritating 3: Severely irritating or corrosive

3A: Corrosi	ive > 1 hr - 4 hr 3	B: Corrosive >3 min < 1 hr 3C: Corrosive < 3min
study no.	proposed rating	source / kind of study / animal species
1		
2		
3		

### **Column D2: Eye Irritation / Corrosion**

0: Not irrita	0: Not irritating 1: Mildly irritating 2: Irritating 3: Severely irritating with irreversible corneal injury						
study no.	proposed rating	source / kind of study / animal species					
1							
2							
3							

### Column D3: Other long term effects (indicate by appropriate letter in box)

Carcinogenic - C	Aspiration haz A	Neurotoxic - N						
Lung injury - L	Reprotoxic – R	Immunotoxic - I						
Mutagenic - M	Photosensitizer - P	Sensitizing - S						
Source/comment:								

# <u>Remarks</u>

ACC2

No data

May well behave partly like piperazine and produce introsoamines in a nitrate rich environment

C1	C2	C3	D1	D2	D3	Date