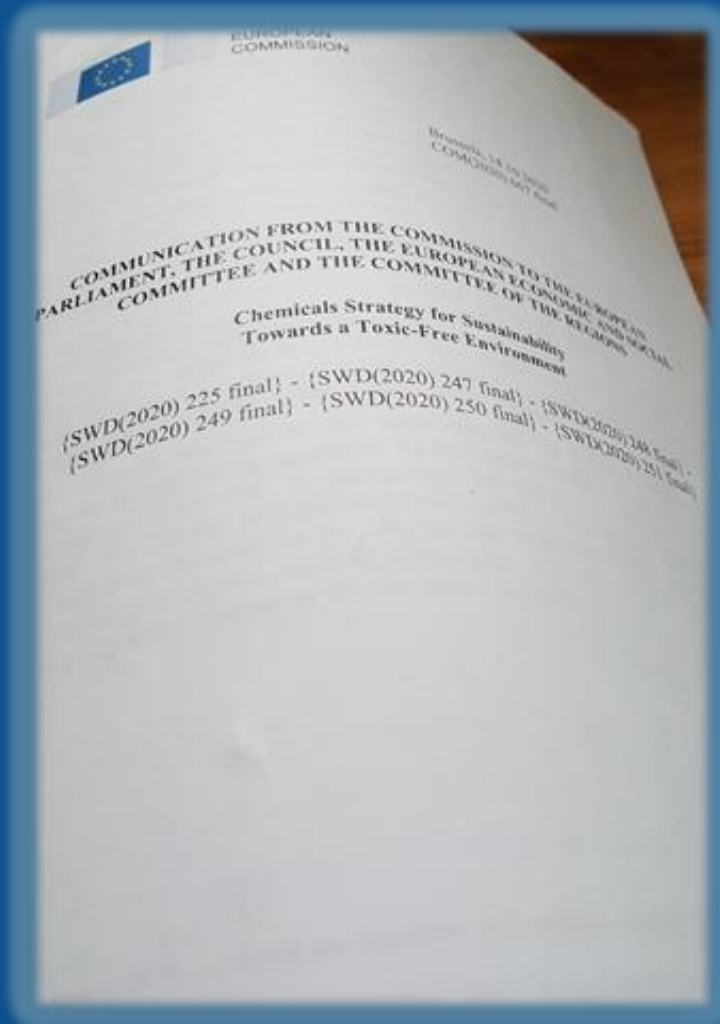




European
Commission



Data, tools and platforms

Information session

Online, 1 June 2022

Andrej Kobe
European Commission



European
Commission

TRANSPARENCY

- Extending open data and transparency principles from the EU food sector to other pieces of chemical legislation

Initiation

- Developing **coordination mechanism** ((P)ACT, expert working group, internal procedures)
- **Promoting grouping** approaches
- CLP amendment – allowing COM to initiate harmonised classification

Allocation

- Proposal for re-allocation of technical and scientific work on chemicals to the EU Agencies
- Proposal for ECHA's founding regulation

Data

- Use **IUCLID** and **IPCHEM**
- **Develop a Common Data Platform on Chemicals**
- **Establish tool for making academic data easily accessible**
- **Remove obstacles for reuse of data and better streamline flow of data**
- **Proposal to allow authorities to commission testing and monitoring of substances**

Methodologies

- Establishment of a **EU repository of health-based limit values**
- CLP amendment – ensuring that CLP is central piece for hazard classification
- Review of definition of nanomaterials

Getting there

One substance, one assessment

CSS actions include...

- *Develop a **common open data platform on chemicals** to facilitate the sharing, access and re-use of information on chemicals coming from all sources*
- *Promote use and reuse of **human and environmental health-based limit values** among risk assessors and managers through a centralized and curated repository*
- *Remove legislative obstacles for the re-use of data and **better streamline** the flow of chemical data between EU and national authorities*
- *Make data available in appropriate **formats and tools** to ensure interoperability*

Chemical data is of different types...

- *Identifiers, groupings*
- *Intrinsic properties, hazard/classification*
- *Presence (in articles) and use, emission, occurrence, exposure*
- *(Hazard and risk) assessments, outcomes incl. limit values*
- *Data on data : controlled vocabularies, methods;
ownership, access...*

... and requires formats & controlled vocabularies* for use, in particular where pulled together from several sources.

*Controlled vocabulary: a consistent way to describe data

Data formats and vocabularies



Build on extensive existing work...

- *OECD Harmonized templates (OHT)*
- *IUCLID*
- *IPChem 'Internal data model': harmonized core set of information mapped from (varied) occurrence data*
- *Assessment (outcomes)*
 - **Varied or unstructured formats but relying on use of pre-defined methods, guidance and tools supporting rapid processing, consistent analysis and reporting**
- *(Common) chemical identifiers*
- *Metadata*

Under 1S1A, joint effort on **common** controlled vocabularies on chemicals and their application on the data managed, to be shared through, and applied by, Common Data Platform



- *A number of legally mandated data flows*
 - **Some streamlining opportunities identified in monitoring data flows**
- *Chemical data flows (re)organization under consideration*
 - **Individual agencies tasked as responsible* for data flows of specific type, supporting dataflow optimization from primary data providers where needed. E.g.**
 - EEA – occurrence data
 - ECHA – intrinsic properties, exposure and use (extend use of IUCLID)

** Not all data flows of certain type require allocation to specific agency. Some changes will require changes to existing legal provisions.*

Repository of health-based limit values

- Unique access point to all human and environment health-based limit values
- Scope : All safety limit values (see right)
 - **by regulators and industry**
 - **EU and international (e.g. WHO, FAO, OECD)**
 - **Based solely on science and those that take into account socio-economic and other considerations**
 - **Values and metadata: who/how have they been derived**

(starting point: EFSA 'OpenFoodTox' database)

- Sustainable/automated and as necessary curated;
- Publicly accessible, machine readable (API)
integral part of the common data platform

Derived No-Effect Level (DNEL)
Predicted No Effect Concentration (PNEC)
Tolerable Upper Intake Level (UL)
Acceptable Operator Exposure Level (AOEL)
Occupational Exposure Limit (OEL)
Maximum Residue Level (MRL)
Maximum Tolerable Dose (MTD)
Population Reference Intake (PRI)
Maximum Tolerable Daily Intake (MTDI)
Derived Minimal Effect Level (DMEL)
Acceptable or Tolerable Daily/Weekly Intake (ADI or TDI/TWI)
Acute reference dose (ARfD)
Acute Acceptable Operator Exposure Level (AAOEL)
Environmental Quality Standards (EQS)
Threshold of Toxicological Concern (TTC)
Average Requirement (AR)
Adequate intake (AI)
Margin of Safety based on hazard and exposure (MoS)

- First version by 2022;

Common Data Platform on Chemicals

Sustainable, long term EU IT infrastructure, an integral feature of EU Green Deal Data Space

*Single common access point to a more complete and comprehensive data and information on chemicals generated at EU level, for all:
authorities, industry, academia, public*

Facilitates sharing, access, re-use and dissemination of information on chemicals through

- *Effective joint access to data from different sources*
- *Provide functionalities and ecosystem of tools to support users*

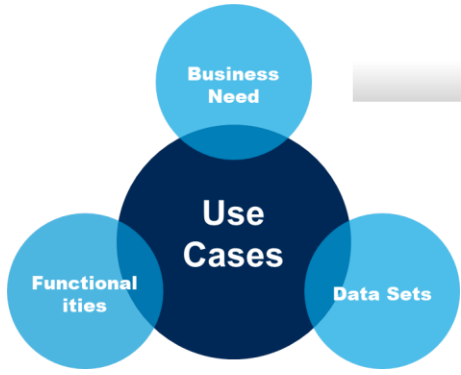
A **feasibility study** was externally commissioned in 2020 to explore the requirements, implications and benefits

- https://final_report_study_platform_chemical_safety_data
*Consortium **Gartner**, Royal HaskoningDHV, Trasys, Milieu and Timelex*



Mapping of sources

&



Development and analysis of Use Cases and sources

Minimum Value Product (MVP)
Minimum Viable Data (MVD)
 +
 further ambition level in future

Platform options

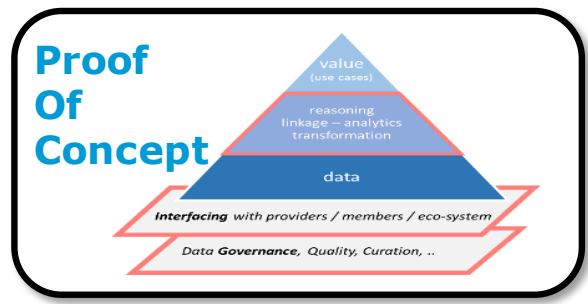
Selected: infrastructure with allowing consolidated or federated access, secure enclaves

Enables MVP+allows future evolution

Analysis of options incl. cost estimates, potential policy, legal and data protection hurdles to overcome

Recommendations

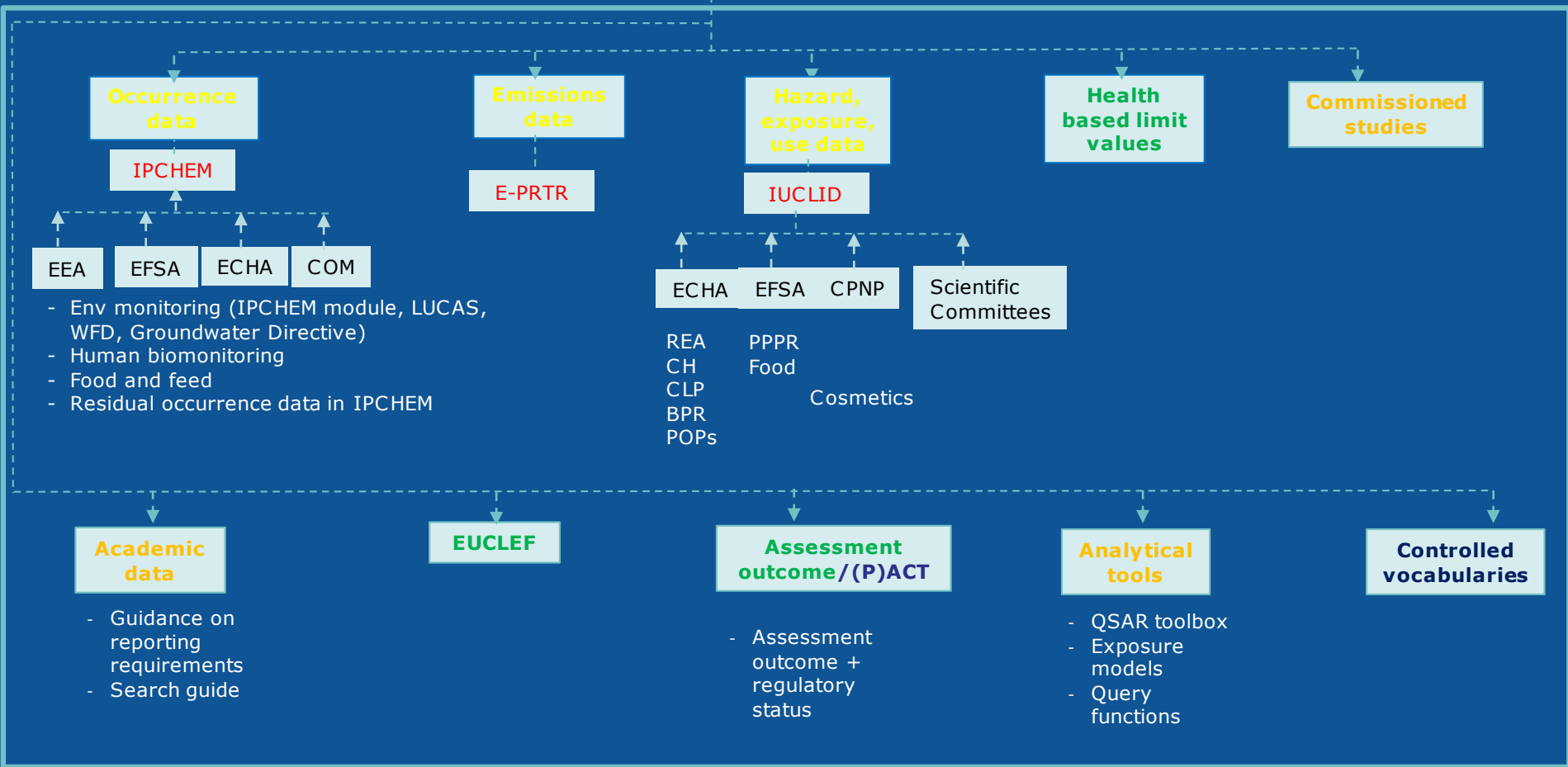
Solution Design specifications IT+governance





User

Common Data Platform on Chemicals





#1 Improve quality of assessment and facilitate 1S1A - Facilitate collaboration and access to all available data to perform an assessment, avoiding duplicate or overlapping assessments under different legislative regimes

#2 Improve safety information and data (incl. C&L) - Industry should be able to reuse existing information and efficiently access different data sources in order to prepare safety instructions.

#3 Group and prioritise chemicals for (common) identification – Improve the effectiveness and efficiency of substance identification as well as the harmonisation, collaboration and prioritisation in the (common) identification of chemicals of concern and their assessment.

#4 Enhance knowledge building through sharing of research - Share research results for the benefit of risk evaluations, impact assessments (health or environmental) and substitutes or sustainability assessments.

#5 Provide and rate methods and standards - Enhance sharing of methods, tools and standards for assessments. (e.g. QSARs)

ECHA

- ECHA_REACH_HAZARD (*Hazard data*)
- ECHA_CLP (*CLP classification*)
- ECHA_REACH_USEEXPO (*use – volumes, wide dispersive use*)
- ECHA_REACH_DUR (*downstream user reports*)
- ECHA_BPR (*hazard, classification, use/exposure, safe use data for biocides*)
- PIC & POP (*identifiers, groupings, restriction*)
- EUCLEF (*legal obligations*)
- (P)ACT (*assessment process data and conclusions*)
- SCIP (*presence of SVHCs in articles*)

EEA

- Air Quality (*Occurrence data*)
- Water Quality + WISE6 (*occurrence data*)
- Emission data (E-PRTR) (*emission data*)

EFSA

- Data warehouse (*Opinions, hazard, occurrence and risk assessments & limits*)
- Data lake (*Hazard and risk data from applicant dossiers*)
- OpenFoodTox (*Hazard and risk assessments & limits*)
- Open EFSA portal (*Assessment process data*)
- Connect EFSA (*Study notifications*)

EMA

- Human medicinal products data (*both ERA and other non-clinical data*)
- Veterinary medicinal products data (*ERA*)
- Maximum residue limit values data and assessments for veterinary products (*limit values*)

Commission

- EMODNET (*use/occurrence data*)
- IPCHEM (*occurrence data*)
- Scientific opinions of SCCS and SCHEER (*risk assessment & limits*)
- E-submission food chain (ESFC) platform (*Identifiers, intrinsic properties (phys/chem, toxicological, microbiological), intended use, risk assessment*)
- EU pesticides database (*Hazard and risk assessments & limits*)
- Cosmetic product notification portal (*Identifiers, Others (presence of certain chemicals, link to the product information file)*)

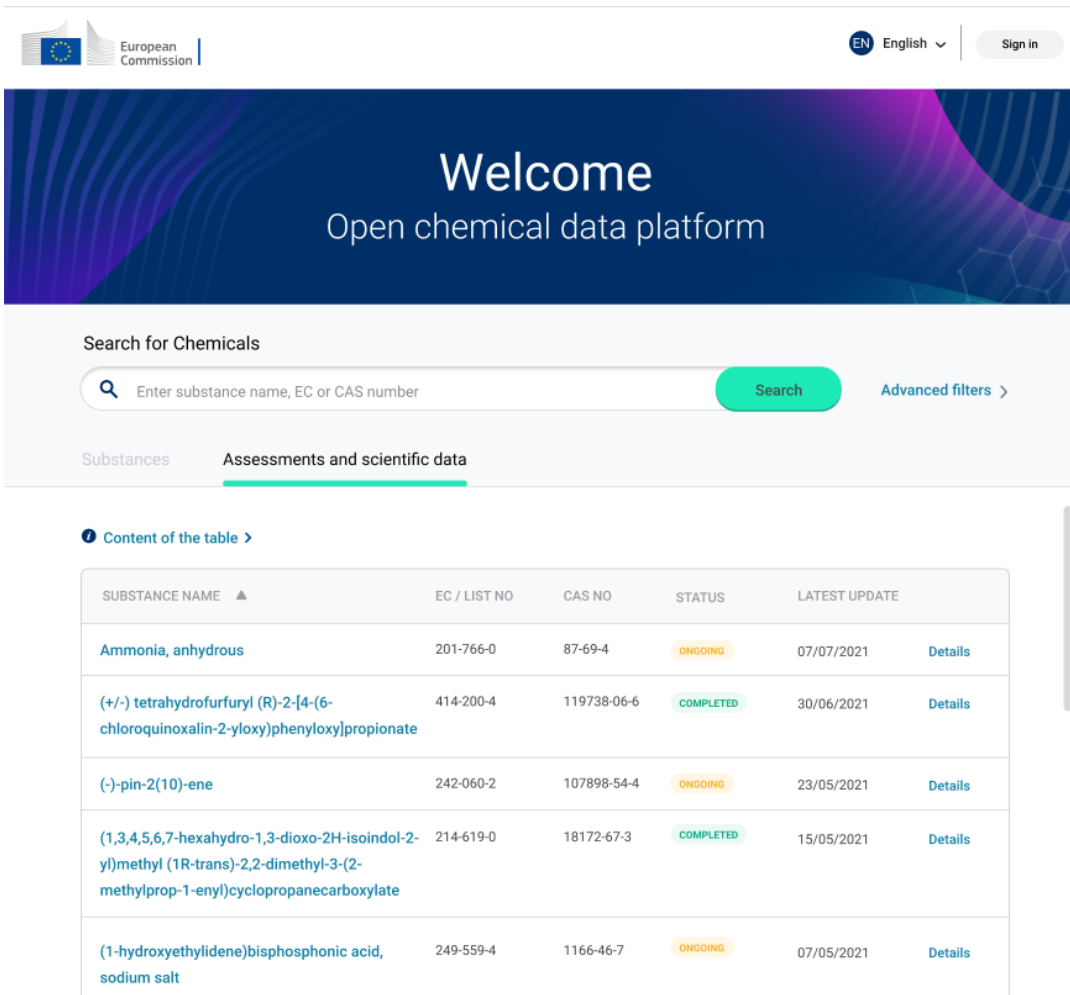
Under development

- Repository of limit values
- Extended (P)ACT

Consideration

- Inclusion of some datasets will require changes in legal provisions, work on formats, effort & timing may differ
- Some further existing data compilations fit well within objectives and may be considered for inclusion e.g. from EU observatory for nanomaterials (EUON)

Webpage

<https://xd.adobe.com/view/7f24b4de-6603-4b93-b7df-3a97e3759c8f-2a77/>


European Commission

EN English Sign in

Welcome

Open chemical data platform

Search for Chemicals

Enter substance name, EC or CAS number Search Advanced filters >

Substances Assessments and scientific data

Content of the table >

SUBSTANCE NAME ▲	EC / LIST NO	CAS NO	STATUS	LATEST UPDATE	
Ammonia, anhydrous	201-766-0	87-69-4	ONGOING	07/07/2021	Details
(+/-) tetrahydrofurfuryl (R)-2-[4-(6-chloroquinoxalin-2-yloxy)phenoxy]propionate	414-200-4	119738-06-6	COMPLETED	30/06/2021	Details
(-)-pin-2(10)-ene	242-060-2	107898-54-4	ONGOING	23/05/2021	Details
(1,3,4,5,6,7-hexahydro-1,3-dioxo-2H-isoindol-2-yl)methyl (1R-trans)-2,2-dimethyl-3-(2-methylprop-1-enyl)cyclopropanecarboxylate	214-619-0	18172-67-3	COMPLETED	15/05/2021	Details
(1-hydroxyethylidene)bisphosphonic acid, sodium salt	249-559-4	1166-46-7	ONGOING	07/05/2021	Details



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EN English ▾
Sign in

← NH₃

Ammonia, anhydrous

🔍

EC number 231-635-3 | CAS number 7664-41-7
Last updated 06/07/2021

📄 Overview

SUBSTANCE

- 📄 General information ▾
- 📄 Classification & Labelling & PBT assessment ▾
- 📍 Substance concentration per location
- 🏭 Manufacture, user & exposure ▾
- 🧪 Physical & Chemical properties ▾
- 🌿 Environmental fate & pathways ▾
- 🌍 Ecotoxicological information ▾
- ⚠️ Toxicological information ▾
- 📄 Analytical methods
- 👤 Threshold limit values
- 📄 Guidance on safe use
- 🔗 Related substances

Overview

N

Ammonia (NH₃) is a compound of nitrogen and hydrogen with the formula NH₃. A stable binary hydride, and the simplest pnictogen hydride, ammonia is a colourless gas with a distinct characteristic of a pungent smell. It is a common nitrogenous waste, particularly among aquatic organisms, and it contributes significantly to the nutritional needs of terrestrial organisms by serving as a precursor to food and fertilizers.

Index number 007-001-00-5
Molecular formula H3N
Type of substance mono-constituent substance

Data sources

Source	Percentage
REACH	13%
EUCLEF	16%
CLP	10%
IPChEM	11%
BPD	5%
Open FoodTox	6%
SCIP	6%
EPRTR	5%
Pesticides	9%
Echa limits	9%
PACT	10%

Ongoing assessments

4

Completed assessments

11

Hazard classification & labelling

Substance concentration per location

31

locations

Similar compounds

13

Chemicals


Threshold limit values

OSHA (TLV)	NIOSH (PEL)	AGGIH (REL)
25 ppm	50 ppm	25 ppm

16



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←

NH₃

Ammonia, anhydrous

EC number 231-635-3 | CAS number 7664-41-7

🔍

Last updated 06/07/2021

📄 Overview

SUBSTANCE

🔍 General information

📄 Substance identity

📄 Administrative information

📄 Regulatory context

📄 Classification & Labelling & PBT assessment

📍 Substance concentration per location

🏭 Manufacture, user & exposure

🧪 Physical & Chemical properties

🌿 Environmental fate & pathways

🌍 Ecotoxicological information


⚠️ Toxicological information

📖 Analytical methods

Substance identity

📄 Download data

🔍 Identification



Name	Ammonia, anhydrous
EC number	231-635-3
EC name	Ammonia, Anhydrous

✕

Source

Organisation: European Chemicals Agency (ECHA)

Record Name: Ammonia, anhydrous

Submitted under: REACH

URL: <https://echa.europa.eu/information-on-chemicals/ci-inventory-database/-/discli/details/216807>

Description: Lorem ipsum dolor...

Contents

- Identification
- Type of substance
- Structural Identifiers
- Substance Identifiers
- Compositions

🔍 Type of substance


Composition	mono-constituent substance
Origin	inorganic

🔍 Structural Identifiers

IUPAC name	Ammonia
Molecular weight	17.03
SMILES notation	N
InChI	InChI=1/H3N/h1H3



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Sign in

Ammonia, anhydrous

EC number 231-635-3 | CAS number 7664-41-7

Last updated 06/07/2021

Overview

SUBSTANCE

- General information
- Classification & Labelling & PBT assessment
- Substance concentration per location
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- Toxicological information
- Analytical methods
- Threshold limit values
- Guidance on safe use
- Related substances

Assessments

The process covers compliance checks and the examination of testing proposals. By consulting the table below, you can find out when has started assessing a particular substance and its progress.

[Content of the table](#)

DECISION TYPE	SCOPE	STATUS	DECISION DATE	DECISION FILE	LATEST UPDATE	SOURCE
CCH	Targeted	ONGOING	-	-	07/07/2021	ECHA
CLH	Testing Proposal	COMPLETED	15/10/2012	j.efsa.2019.5868		Contact johnmiller@ipchem.eu
TPE	Testing Proposal	ONGOING	-	-	23/05/2021	IPCHEM
CCH	Targeted	FOLLOW-UP	11/04/2020	CCH-D-000048-767/F	19/04/2021	HBM4EU Details

Showing 4 of 4 results



← | CLH

Source [EFSA](#)[Download data](#) ▾

Identifiers of the assessment

Concern	Health risk of ammonium released from water filters
Status	COMPLETED
Outcome	Exposure estimates and their relevance for human health within the specified concentration range (0.5-5 mg/L)
Decision type	CLH
Legislation	No 1935/2004 (27 October 2004)
On request from	European Commission
Correspondence:	contam@efsa.europa.eu

Activity dates

Approved	15/10/2012
Published date	19/10/2012

Conclusion

Estimated exposure in water for adults	0.014 - 0.14 mg/kg b.w. per day
Estimated exposure in water for infants	0.10 - 1.0 mg/kg b.w.per day
Estimated exposure in water for childrens	0.054-0.54 mg/kg b.w. per day

Opinion outcome and related files

CLH Report	CLH_Volume_1_2012-10-15.pdf
Decision file	j.efsa.2012-10-15.pdf
Comment	The European Commission (EC) asked the European Food Safety Authority (EFSA) for scientific assistance regarding the possible impact on human health of exposure to ammonium released from water filter cartridges.
Date of opinion	15/10/2012
Citing Literature	7
Submitter	EFSA, Parma, Italy

Threshold limit values

[Dow](#)

Workspace exposure limits

OSHA	The legal airborne permissible exposure limit (PEL) is 50 ppm , averaged over an 8-hour work shift.
NIOSH	The recommended airborne exposure limit (REL) is 25 ppm averaged over a 10-hour work shift and 35 ppm , not to be exceeded during any 15-minute work period.
AGGIH	The threshold limit value (TLV) is 25 ppm averaged over an 8-hour workshift and 35 ppm as a STEL (short-term exposure limit).
IDLH LEVEL	300 ppm
ERPG-1	25 ppm
ERPG-2	150 ppm
ERPG-3	1,500 ppm

- Platform development will rely as much as possible on **building blocks** from EU data space and the chemical sector (IUCLID)
- Data governance: **data providers** responsible for preparation of interoperable datasets and access to them (or consistent data flows)
- Expansion and evolution:

MVD is an initial list; there is no inherent restriction on inclusion of **further relevant datasets**

Governance with all stakeholders is crucial for sustained success, addressing present and identifying future use cases with associated needs for tools, platform functionalities and data

- **In 2022, detailed implementation plan** is being drafted by the **anticipated host (ECHA)** in close cooperation with other agencies and Commission services, to entail:
 - Technical blueprint and operational steps
 - Review and confirmation of use cases and MV data
 - Resource estimations
 - Governance setup
- **MVP go-live foreseen for 2025, some components may be available before**
- **Platform success will also depend on:**
 - Alignment with processes emerging under 1S1A
 - Removal of legislative barriers to data sharing
 - Coordination/collaboration of source data holders

Thank you

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andrej.kobe@ec.europa.eu

Common Data Portal in support of 1S1A



'analytical' Tools
(QSAR Toolbox, data
analytics, Query
functions, exposure
models)

Hosting data
for others

Control vocabularies,
dictionaries, formats

Academic
chemicals data

Status on Regulatory
Processes
Extended (P)ACT
Extended EUCLEF

Unique study
identification

Repository of
health limit
values

Outcomes of the
assessments

Emission data
E-PRTR

Central database(s) with regulatory submissions
of intrinsic properties, C&L, uses, SCIP database,
etc



Occurrence data

