Substance Identification and Naming Convention for Hydrocarbon Solvents under REACH

Contents

1. Background for solvent new identification
2. Hydrocarbon solvents naming convention

Creation of

SUBSTANCE IDENTIFICATION

Hydrocarbon Solvents - Background

Hydrocarbon Solvents:

- Composed only from hydrogen and carbon
- Carbon number range ~ C5-C20
- Are usually complex substances (UVCBs), but may also be monoconstituent and multiconstituent substances
- Highly refined as manufacturing of HC solvents require specific processing steps to address customers needs (boiling range, evaporation rate, solvency power)
- Need to meet regulatory and SHE requirements
- Typically have a narrow distillation range
- Derived from petroleum, coal, natural gas or organic material

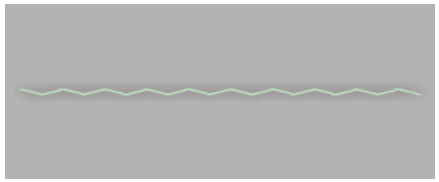
Physical/Chemical properties

- Related to carbon number e.g. volatility and flammability

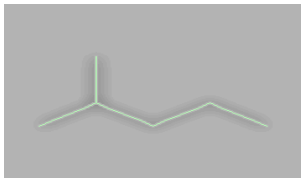
Limited Compositional Elements
All Constituents Defined by Four Structures

C5

N-paraffins

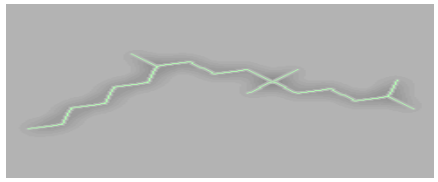


C20

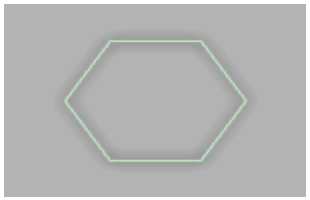


C6

Iso-paraffins

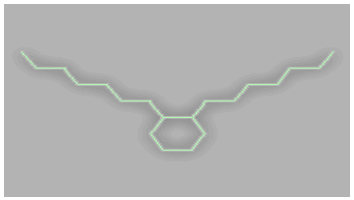


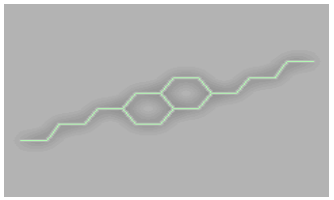
C20



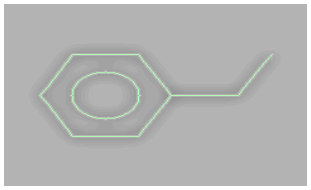
C6

Cyclics



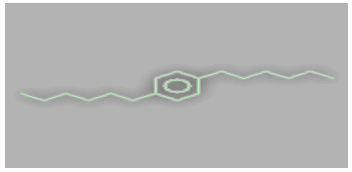


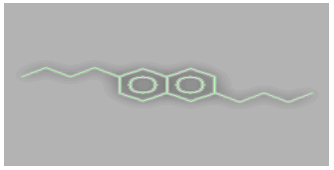
C20



C8

Aromatics





C18

Solvent Complexity Due to Increasing Numbers of Isomers with Increasing Carbon Number

Carbon number	N-paraffins	Iso-paraffins	cyclics	aromatics
C5	1	3		
C6	1	5	1	
C7	1	9	1	
C8	1	18	4	4
C9	1	35	8	8
C10	1	75	22	22
C11	1	159	51	51
C12	1	355	136	136
C13	1	802	335	335
C14	1	1858	871	871
C15	1	4347	2217	2217
C16	1	10359	5749	5749
C17	1	24894	14837	14837
C18	1	60523	38636	38636
C19	1	148284	100622	
C20	1	366319	263381	

- Characterization only possible by molecule type per carbon range
- Composition variable but not unknown

Background to solvent naming

Since late 1980's HSPA has been working on common rules and approach for solvents identification for a common environmental classification and voluntary participation to OECD HPV project

Prior to REACH registration: Assessment of hydrocarbon solvents

- HC solvents are used in a very broad spectrum of applications: coatings, process fluids, agrochemicals, cleaning, household, pharmaceutics, cosmetics, intermediates…..
- EINECS descriptions exists for a number of hydrocarbon substances derived from petroleum refining and chemical conversion. These descriptions are overly broad to describe hydrocarbon solvent substances according to needs of Reach
- Several EINECS# for a similar substance
- Some solvent standards exist, but there was no common naming for hydrocarbon solvent substances indicating their chemical composition.

Need for better characterisation of HC solvents

Need to adopt a consistent substance identification system

Hydrocarbon solvents naming shall fulfil the criteria within the REACH substance identification guidance.

As an outcome of this exercise, a common naming system has been developed to identify similar substances.

Examples of CAS vs chemical identity

C9-14 Aliphatics (2-25% aromatics)	Hydrocarbons, C9-C10, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)	927-344-2	→	64742-82-1	Naphtha (petroleum), hydrodesulfurized heavy
C9-14 Aliphatics (2-25% aromatics)	Hydrocarbons, C10-C13, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)	919-164-8	→	64742-82-1	Naphtha (petroleum), hydrodesulfurized heavy
C9-14 Aliphatics (2-25% aromatics)	Hydrocarbons, C8-12, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)	928-136-4	→	64742-82-1	Naphtha (petroleum), hydrodesulfurized heavy; Low boiling point hydrogen treated naphtha
C9-14 Aliphatics (2-25% aromatics)	Hydrocarbons, C9-C12, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)	919-446-0	→	64742-82-1	Naphtha (petroleum), hydrodesulfurized heavy
			→	64742-88-7	Solvent naphtha (petroleum), medium aliphatic
C9-14 Aliphatics (2-25% aromatics)	Hydrocarbons, C11-C14, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)	925-653-7	→	64742-81-0	Kerosine (petroleum), hydrodesulfurized

EINECS 265-149-8

CAS 64742-47-8

Distillates (petroleum), hydrotreated light A complex combination of hydrocarbons obtained by treating a petroleum fraction with hydrogen in the presence of a catalyst. It consists of hydrocarbons having carbon numbers predominantly in the range of C9 through C16 and boiling in the range of approximately 150°C to 290°C (302°F to 554°F).

EINECS 265-150-3 Low boiling point hydrogen treated naphtha

CAS 64742-48-9 Naphtha (petroleum), hydrotreated heavy

A complex combination of hydrocarbons obtained by treating a petroleum fraction with hydrogen in the presence of a catalyst. It consists of hydrocarbons having carbon numbers predominantly in the range of C6 through C13 and boiling in the range of approximately 65°C to 230°C (149°F to 446°F).

C9-14 Aliphatics (<=2% aromatic)	Hydrocarbons, C9-C11, n-alkanes, isoalkanes, cyclics, < 2% aromatics	919-857-5	→	64742-48-9	Naphtha (petroleum), hydrotreated heavy
			→	64771-72-8	Paraffins (petroleum), normal C5-20
C9-14 Aliphatics (<=2% aromatic)	Hydrocarbons, C9-C10, n-alkanes, isoalkanes, cyclics, < 2% aromatics	927-241-2	→	64742-48-9	Naphtha (petroleum), hydrotreated heavy
			→	64742-49-0	Naphtha (petroleum), hydrotreated light
C9-14 Aliphatics (<=2% aromatic)	Hydrocarbons, C9-C11, isoalkanes, cyclics, < 2% aromatics	920-134-1	→	64742-48-9	Naphtha (petroleum), hydrotreated heavy
			→	68551-16-6	Alkanes, C9-11 iso
C9-14 Aliphatics (<=2% aromatic)	Hydrocarbons, C10-C13, n-alkanes, isoalkanes, cyclics, < 2% aromatics	918-481-9	→	64742-48-9	Naphtha (petroleum), hydrotreated heavy
C9-14 Aliphatics (<=2% aromatic)	Hydrocarbons, C10-C13, isoalkanes, cyclics, < 2% aromatics	918-317-6	→	64742-48-9	Naphtha (petroleum), hydrotreated heavy
			→	68551-19-9	Alkanes, C12-14-iso-
			→	90622-57-4	Alkanes, C9-12-iso-
			→	68551-17-7	Alkanes, C10-13 iso
C9-14 Aliphatics (<=2% aromatic)	Hydrocarbons, C11-C14, n-alkanes, isoalkanes, cyclics, < 2% aromatics	926-141-6	→	64742-47-8	Distillates (petroleum), hydrotreated light
			→	64742-48-9	Naphtha (petroleum), hydrotreated heavy
C9-14 Aliphatics (<=2% aromatic)	Hydrocarbons, C13-C15, n-alkanes, isoalkanes, cyclics, < 2% aromatics	917-488-4	→	64742-47-8	Distillates (petroleum), hydrotreated light
C9-14 Aliphatics (<=2% aromatic)	Hydrocarbons, C12-C16, isoalkanes, cyclics, < 2% aromatics	927-676-8	→	64742-47-8	Distillates (petroleum), hydrotreated light
C9-14 Aliphatics (<=2% aromatic)	Hydrocarbons, C12-C15, n-alkanes, isoalkanes, cyclics, < 2% aromatics	920-107-4	→	64742-47-8	Distillates (petroleum), hydrotreated light
			→	64742-48-9	Naphtha (petroleum), hydrotreated heavy
C9-14 Aliphatics (<=2% aromatic)	Hydrocarbons, C11-C14, isoalkanes, cyclics, < 2% aromatics	927-285-2	→	64742-47-8	Distillates (petroleum), hydrotreated light
			→	90622-58-5	Alkanes, C11-15-iso-
			→	68551-17-7	Alkanes, C10-13-iso-
			→	68551-19-9	Alkanes, C12-14 iso
C9-14 Aliphatics (<=2% aromatic)	Hydrocarbons, C10-C12, isoalkanes, < 2% aromatics	923-037-2	→	90622-57-4	Alkanes, C9-12-iso-
			→	64741-65-7	Naphtha (petroleum), heavy alkylate
C9-14 Aliphatics (<=2% aromatic)	Hydrocarbons, C11-C12, isoalkanes, < 2% aromatics	918-167-1	→	90622-58-5	Alkanes, C11-15-iso-
			→	90622-57-4	Alkanes, C9-12-iso-
			→	64741-65-7	Naphtha (petroleum), heavy alkylate
C9-14 Aliphatics (<=2% aromatic)	Hydrocarbons, C11-C13, isoalkanes, < 2% aromatics	920-901-0	→	90622-58-5	Alkanes, C11-15-iso-
C9-14 Aliphatics (<=2% aromatic)	Hydrocarbons, C10-C13, n-alkanes, < 2% aromatics	929-018-5	→	93924-07-3	Alkanes, C10-14
			→	64771-72-8	Paraffins (Petroleum), normal C5-20

HYDROCARBON SOLVENTS NAMING CONVENTION

The identification and naming system basis

- Guidance for identification and naming of substances under REACH
- Products of similar composition (carbon number range and chemical structures) and similar use should be the same substance
- One hydrocarbon solvent substance = one classification to the extent possible

Three types of substances have been defined by REACH

1) Mono-constituent substances, which consist for more than 80% out of one main component.

They are described by the name of this single main component e.g. n-pentane, n-hexane, n-decane

2) Defined multi-constituent substances, in which the main constituents are present in a concentration between 10 and 80%.

The composition must be known, fixed and predictable; more than one constituent is relevant for the identification.

3) Unknown or Variable composition, Complex reaction products or Biological materials (UVCB) substances.

As hydrocarbon solvents can be complex substances, a number of hydrocarbon solvents meet the criteria for UVCB substances as the number of chemical constituents is relatively large and the composition of chemical components is variable.

Identification and naming convention

For UVCB hydrocarbon solvents:

1. **"Hydrocarbons" will be the first part of the name** to recognize their specific chemical character.
2. **The carbon number range** (which must at least include 80% of the components of the substance) determined by GC/MS an equivalent test method.
3. **The description of the hydrocarbon structures** present (PINA): n-paraffins (n-alkanes), isoparaffins (isoalkanes), saturated cyclics (naphthenes) and aromatics. The first three are mentioned when present in the substance at a level between 10 and 80%. Aromatic-containing substances are differentiated based on aromatic content (e.g., < 2%, 2-25%, 100%)
4. **Components with specific toxicology or classification** will be mentioned, using the classification cut-off as an indication level (according to EU DSD (Dangerous Substances Directive) guidance) E.g. n-hexane (5 %), Naphthalene (1 %), Benzene (0.1 %)

Note:The HSPA naming description can also be used for solvents belonging to the first two types of substances (mono-constituents and defined multi constituents

Example of substance naming: A Regular White spirit

A regular white spirit's composition is analyzed by Gas Chromatography (GC) and Mass Spectrophotometry (MS). Also with GC the carbon split was determined as follows:

Carbon number	C8	C9	C10	C11	C12	C13
Amount in %	1	10	40	42	6	1

GC analysis shows a total aromatic content of 19% and a benzene content of 0.0001%. With MS the non aromatic fraction is separated into a naphthenic (saturated cyclics) fraction of 33%, a normal paraffin (n-alkanes) fraction of 22% and an isoparaffin (isoalkanes) fraction of 26%.

Naming of the substance:

1. The substance consists of H and C. The name will start with "Hydrocarbons".

2. Carbon range:

The major components will be indicated by giving the carbon number range. The determined/given components must cover at least 80% of the total composition and individual components bigger than 10% must be mentioned and the variation of the composition is taken into account. Individual components below 10% are not described unless they trigger a health or environmental classification. The substance name becomes "Hydrocarbons, C9-C11".

3. Component split:

Determine the component split by GC/MS into normal n-alkanes, isoalkanes, cyclics and aromatics. For the component split we again start from the RIP 3.10 rule, specifying that each component equal or above 10% must be mentioned and that at least 80% of the total composition must be covered. Each of the possible four component groups (see above) is present at more than 10% and must thus be mentioned in the substance name. So the name must include n-alkanes, isoalkanes, cyclics and aromatics. According to naming convention substance name is now "Hydrocarbons, C9-C11, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)".

4. Components with specific toxicology or classification:

Components which trigger a specific classification or labeling are mentioned if present and if measured above the cut-off limit.

Benzene leads to classification if present at a level of or above 0.1%. The concentration is however below the regulatory cut-off point so it will nor be part of the name. Name remains: "Hydrocarbons, C9-C11, n-alkanes/isoalkanes/cyclics/aromatics (2-25%)".

Final name for REACH registration: Hydrocarbons, C9-C11, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)

Example of difference in substance identification between EINECS and hydrocarbon solvents naming

An example of the actual difference in product description for a substance, depending on using the EINECS number or the Hydrocarbons naming convention, is presented in the naming convention as Example 1.

The chosen product is a typical de-aromatised white spirit, with following composition:

Components	**amount**
Normal paraffins	25%
Isoparaffins	25%
Cyclics	49.6%
Aromatics	0.4%

Carbon number	C8	C9	C10	C11	C12	C13
Amount in %	1	10	40	42	6	1

In the RIP 3.10 guidelines, it is indicated that only the components present in an amount above 10% must be given and that the given substance description must at least include 80% of the determined composition. In this example only normal paraffins, isoparaffins and cyclics with a carbon number of C9, C10 and C11 should be provided.

Difference depending on the chosen naming description:

	EINECS number	**HSPA convention**
Substance description	265-150-3 Naphtha (petroleum) Hydrotreated heavy	**Hydrocarbons, C9-11 n-alkanes, isoalkanes, cyclics, <2% aromatics**
Specified carbon range	C6 - C13	**C9 - C11**
Specified boiling range	65 - 230 °C	**160 - 190 °C**
Aromaticity	**Not addressed**	**Addressed**

Registration in practice

Relationship between the naming convention (substances) and groups of similar substances (categories)

- “Similar substances” are grouped into categories for hazard characterization.
- “Same substances” fall within the compositional parameters defined by the naming convention.

A chemical category is a group of chemicals whose physicochemical and toxicological properties are likely to be similar or to follow a regular pattern as a result of structural similarity.

As shown in the example below, hydrocarbon solvent categories were based on common constituents with similar carbon numbers. The differentiating characteristics are carbon number range, aromatic content, and the presence of n-hexane and/or naphthalene at toxicologically relevant levels.

Because the category members have structural similarities, there are predictable patterns in physicochemical properties, resulting in similarities in human and environmental health effects and environmental fate properties.

Thus, hazards for substances in each category can be characterized on a generic basis using data from studies of representative substances.

Hydrocarbon Solvents Consortium

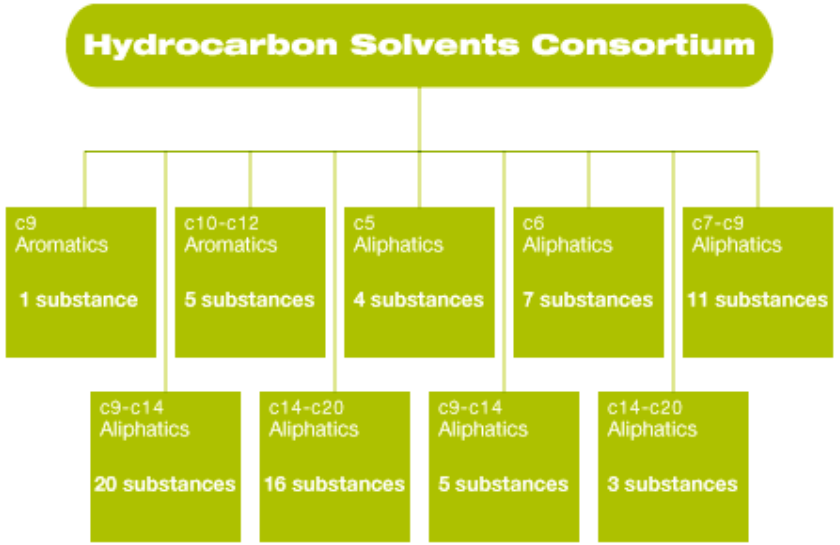
The objective of the consortium is to undertake the collective activities related to the registration of Hydrocarbon Solvents under REACH, including sharing of relevant research information.

Consortium structure:

Steering Committee, Technical Committee

9 categories/ ~80 substances

Information change with Hydrocarbon solvent producer Association HSPA naming convention



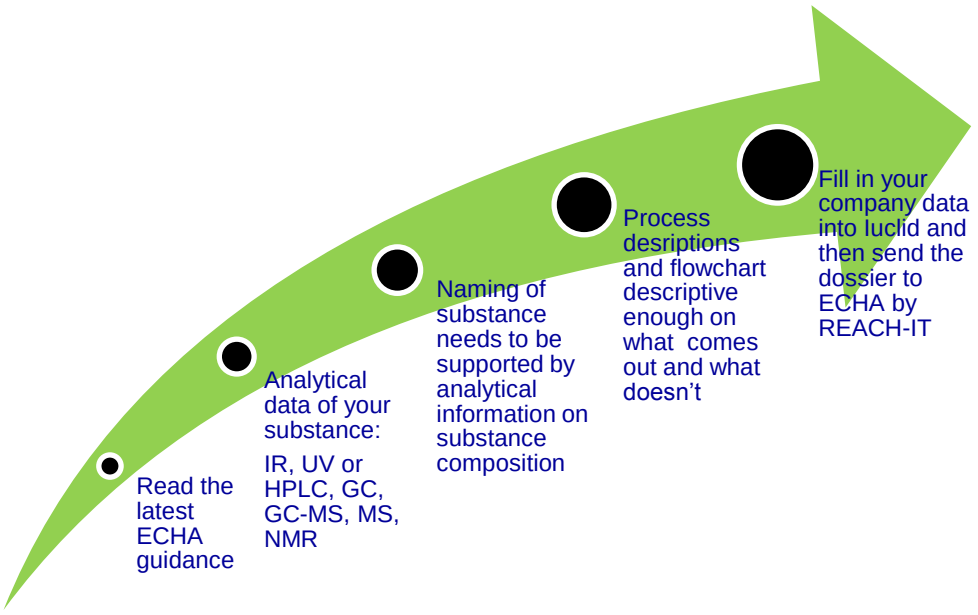
Information required for SUBSTANCE IDENTIFICATION

Basis:

Any information suitable and necessary to allow ECHA to verify the the composition and the name of the substance

A package has been created by Hydrocarbon Producers Association HSPA and Hydrocarbon Solvents Consortium HCSC to assist SIEF and consortia members in naming their substances ”Substance Identification and Naming Convention for Hydrocarbon Solvents under REACH”

The package includes a list of the substances in the consortium.



Summary

Hydrocarbon solvents have common constituents. These similar constituents can be defined using the naming convention and grouped into categories. Because the constituents are similar, the solvents have similar physical and chemical properties which result in similar hazards. As a consequence, the hazards can be characterized on a generic basis.

This approach aims at:

- Facilitating identification of the substances.
- Facilitating identification of sameness of substances
- Providing more clarity for authorities, for registrants and for the market
- Allowing more targeted hazard characterization and risk assessments
- Avoiding misperceptions and misclassifications

Thank You!

More information available

Hydrocarbon Solvents consortium HCSC — HCSC website

Hydrocarbon Solvents Producer Association HSPA

European solvents industry Group ESIG — ESIG website