

Substance identification and naming
convention for hydrocarbon solvents
under REACH

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Substance identification and naming convention for hydrocarbon solvents under REACH

Introduction:

REACH requires a clear and logical substance description. Substance identification is a key component in pre-registration, SIEF and potential consortia formation, and subsequent registration. In order to facilitate appropriate registration of hydrocarbon solvents, the Hydrocarbon Solvents Producers Association (HSPA) has conducted an in-depth assessment of hydrocarbon solvents in order to better characterize its substances and adopt a consistent substance identification system.

The purpose of this letter is to explain the approach followed by HSPA to describe hydrocarbon solvents under REACH requirements and to provide guidelines on the use of the hydrocarbon solvent naming convention as part of the pre-registration process.

Approach:

The European Inventory of Existing Commercial Substances (EINECS) descriptions and numbers have been used historically to identify chemical substances. EINECS descriptions exist for a number of hydrocarbon substances derived from petroleum refining and chemical conversion. However, these descriptions are overly broad to describe hydrocarbon solvent substances as solvents have narrower hydrocarbon ranges, different classifications and different processing.¹ A more focused and narrow definition is therefore required. In attachment to this letter ([attachment 1](#) - page 6), you will find an example highlighting the differences that exist today between the EINECS description and the Hydrocarbon solvents, here for a de-aromatised white spirit.

HSPA more precisely defines hydrocarbon solvents by establishing criteria within the REACH substance identification guidance. As an outcome of this exercise, a common naming system has been developed to identify properly similar substances.

¹ RIP 3.10 point 4.3.1.1

Benefits:

This approach provides significant benefits to the registration of hydrocarbon solvents by:

- Facilitating identification of the substances.
- Facilitating identification of sameness of substances and as such facilitating SIEF formations.
- Providing more clarity for authorities, for registrants (other than HSPA members) and for the market
- Allowing more targeted hazard characterization and risk assessments
- Avoiding misperceptions and misclassifications.

The approach is fully compatible with REACH requirements.

Identification and naming convention:

The identification and naming system is based on the following:

- The RIP 3.10 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.
- It is in line with the HPV (High Production Volume) project, owned by OECD, for read across purposes (see attachment 4).

Three types of substances have been defined by REACH in the RIP 3.10²:

1) Mono-constituent substances, which consist for more than 80% out of one main component.³

They are described by the name of this single main component.

Examples are n-pentane, n-hexane, n-decane, and toluene.

2) Defined multi-constituent substances, in which the main constituents are present in a concentration between 10 and 80%.⁴

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

² RIP3.10 chapter 4

³ RIP 3.10 subchapter 4.2.2

⁴ RIP 3.10 chapter 4.3

These substances will be described as specified in RIP 3.10 by the chemical name and identifiers of the substance as such.

Example given in RIP 3.10: technical xylene, consisting out of m-xylene, p-xylene and o-xylene, will be described as "mixture of p, m and o-xylene".

3) **Unknown or Variable composition Complex reaction products or Biological materials (UVCB) substances.**⁵

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

The convention agreed upon to describe UVCB hydrocarbon solvents is the following:

- a) **"Hydrocarbons"** will be the first part of the name to recognize their specific chemical character.
- b) **The carbon number range** (which must at least include 80% of the components of the substance) determined by Gas Chromatography (GC) or an equivalent test method.
- c) **The description of the hydrocarbon structures** present or the PINA structure: n-paraffins (or n-alkanes), isoparaffins (or isoalkanes), saturated cyclics (or naphthenes) and aromatics. The first three are mentioned when present in the substance at a level between 10 and 80%. Aromatics will be indicated as per HPV category.
- d) **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).

Detailed examples can be found under [attachment 2](#) - page 7.

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) in order to define if they fit into one of the existing HSPA naming categories. If they do so, they can join the HSPA consortium and benefit from read across for data on the corresponding category.

⁵ RIP 3.10 subchapters 4.3.2.1 & 4.3.2.2

Attachment 1:

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

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

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

<u>Components</u>	<u>amount</u>
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	not given, but +_ 160 - 190 °C
Aromaticity	Not addressed	Addressed
Allowed hazard classification	R11, R20,R45, R46, R48, R63 R38, R65, R66, R67, R51/53	R10, R65, R66

Attachment 2:

Example of substance naming for hydrocarbon solvents: regular white spirit.

A regular white spirit's composition is analyzed by Gas Chromatography (GC) and Mass Spectrophotometry (MS).

GC analysis revealed a total aromatic content of 19% and a benzene content of 0.0001%. 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

With MS the non aromatic fraction could be 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:

a) Substance nature:

The product is a liquid, used specifically as solvent, with resulting purity restrictions and specific manufacturing processes. The chemical nature of the solvent is clearly hydrocarbon, so the name will start with the generic description "**Hydrocarbons**".

b) Carbon range:

The major components will be indicated by giving the carbon number range. For this we use the rule described in RIP 3.10. The determined/given components must cover at least 80% of the total composition and individual components bigger than 10% must be mentioned. Individual components below 10% are considered as impurities and must not be described unless they trigger a health or environmental classification.

In this case we do not know the exact constituents of each carbon number range, but even if the C8, C12 and C13's are related to one single component, they do not reach the 10% required in RIP 3.10. So there is no need to mention them. The remaining components cover more than 80% of the composition: the sum of C9, C10 & C11 makes 92%. Since the exact composition of each fraction is impossible to determine we consider each carbon number range as one component, which must be reflected in the name.

The substance name becomes "Hydrocarbons, **C9-C11**".

c) Component split:

The best we can do with actual analytical methods is to determine the component split by 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. We also consider the existing HPV classification, which splits the hydrocarbons in defined groups.

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.

Regular white spirit is actually classified in the HPV table under the category "C9-C14 Aliphatics (2-25% aromatics)". To highlight the relationship with the existing HPV definition, we decided to specify the aromatic range according to this guideline (2-25%). Substance name is now "Hydrocarbons, C9-C11, **n-alkanes, isoalkanes, cyclics, aromatics (2-25%)**".

d) 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.

In this case, benzene has been measured. This component leads to classification if present at a level of or above 0.1%. The concentration is however below the regulatory cut-off point so no need to mention the component in the naming.

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%)

Other Examples:

Technical hexane is: "Hydrocarbons, C6, n-alkanes/isoalkanes/cyclics, n-hexane (5-80%)".

Dearomatised white spirit is: "Hydrocarbons, C9-C11, n-alkanes, isoalkanes, cyclics, <2% aromatics.

Attachment 3:

Example of info required in a pre-registration document:

To be completed.

Attachment 4:

Defined substances per HPV category:

You can find below the list of the until now determined hydrocarbon substances, grouped by HPV category:

HSPA Category	HSPA Substance Name	Reach Registration provisional EC No.
C9 Aromatics	Hydrocarbons, C9, aromatics	918-668-5
C10-12 Aromatics	Hydrocarbons, C10, aromatics, >1% naphthalene	919-284-0
C10-12 Aromatics	Hydrocarbons, C10, aromatics, <1% naphthalene	918-811-1
C10-12 Aromatics	Hydrocarbons, C10-C13, aromatics, <1% naphthalene	922-153-0
C10-12 Aromatics	Hydrocarbons, C10-C13, aromatics, >1% naphthalene	926-273-4
C9-14 Aliphatics (2-25% aromatics)	Hydrocarbons, C9-C10, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)	927-344-2
C9-14 Aliphatics (2-25% aromatics)	Hydrocarbons, C10-C13, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)	919-164-8
C9-14 Aliphatics (2-25% aromatics)	Hydrocarbons, C8-12, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)	928-136-4
C9-14 Aliphatics (2-25% aromatics)	Hydrocarbons, C9-C12, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)	919-446-0

C9-14 Aliphatics (2-25% aromatics)	Hydrocarbons, C11-C14, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)	925-653-7
C14-20 Aliphatics (2-30% aromatic)	Hydrocarbons, C14-C18, n-alkanes, isoalkanes, cyclics, aromatics (2-30 %)	920-360-0
C14-20 Aliphatics (2-30% aromatic)	Hydrocarbons, C16-C20, n-alkanes, isoalkanes, cyclics, aromatics (2-30 %)	919-006-8
C5 Aliphatics	Normal-Pentane	203-692-4

C5 Aliphatics	ISO-Pentane	201-142-8
C5 Aliphatics	Cyclopentane	206-016-6
C5 Aliphatics	Hydrocarbons, C5, n-alkanes, isoalkanes	921-577-3
C6 Aliphatics	Normal-Hexane	203-777-6
C6 Aliphatics	Hydrocarbons, C6, isoalkanes, <5% n-hexane	931-254-9
C6 Aliphatics	Hydrocarbons, C6, n-alkanes, isoalkanes, cyclics, n-hexane rich	925-292-5
C6 Aliphatics	Hydrocarbons, C6-C7, isoalkanes, cyclics, < 5% n-hexane	926-605-8
C6 Aliphatics	Hydrocarbons, C5-C7, n-alkanes, isoalkanes, n-hexane rich	930-397-4
C7-9 Aliphatics	Hydrocarbons, C7, n-alkanes, isoalkanes, cyclics	927-510-4
C7-9 Aliphatics	Hydrocarbons, C6-C7, n-alkanes, isoalkanes, cyclics, > 5% n-hexane	924-168-8

C7-9 Aliphatics	Hydrocarbons, C6-C7, n-alkanes, isoalkanes, cyclics, < 5% n-hexane	921-024-6
C7-9 Aliphatics	Hydrocarbons, C7-C9, n-alkanes, isoalkanes, cyclics	920-750-0
C7-9 Aliphatics	Hydrocarbons, C6-C10, n-alkanes, isoalkanes, > 5% n-hexane	920-191-2
C7-9 Aliphatics	Hydrocarbons, C7-C9, isoalkanes	921-728-3
C7-9 Aliphatics	Hydrocarbons, C7-C8, cyclics	927-033-1
C7-9 Aliphatics	Methyl cyclohexane	203-624-3
C7-9 Aliphatics	Normal-Heptane	205-563-8
C7-9 Aliphatics	Iso-Heptane	250-610-8
C7-9 Aliphatics	Normal-Octane	203-892-1
C7-9 Aliphatics	Iso-Octane	208-759-1
C7-9 Aliphatics	Nonane	203-913-4
C9-14 Aliphatics (<=2% aromatic)	Hydrocarbons, C9-C11, n-alkanes, isoalkanes, cyclics, < 2% aromatics	919-857-5
C9-14 Aliphatics (<=2% aromatic)	Hydrocarbons, C9-C10, n-alkanes, isoalkanes, cyclics, < 2% aromatics	927-241-2
C9-14 Aliphatics (<=2% aromatic)	Hydrocarbons, C9-C11, isoalkanes, cyclics, < 2% aromatics	920-134-1

C9-14 Aliphatics (<=2% aromatic)	Hydrocarbons, C10-C13, n-alkanes, isoalkanes, cyclics, < 2% aromatics	918-481-9
C9-14 Aliphatics (<=2% aromatic)	Hydrocarbons, C10-C13, isoalkanes, cyclics, < 2% aromatics	918-317-6
C9-14 Aliphatics (<=2% aromatic)	Hydrocarbons, C11-C14, n-alkanes, isoalkanes, cyclics, < 2% aromatics	926-141-6
C9-14 Aliphatics (<=2% aromatic)	Hydrocarbons, C13-C15, n-alkanes, isoalkanes, cyclics, < 2% aromatics	917-488-4
C9-14 Aliphatics (<=2% aromatic)	Hydrocarbons, C12-C15, n-alkanes, isoalkanes, cyclics, < 2% aromatics	920-107-4
C9-14 Aliphatics (<=2% aromatic)	Hydrocarbons, C11-C14, isoalkanes, cyclics, < 2% aromatics	927-285-2
C9-14 Aliphatics (<=2% aromatic)	Hydrocarbons, C10-C12, isoalkanes, < 2% aromatics	923-037-2
C9-14 Aliphatics (<=2% aromatic)	Hydrocarbons, C11-C12, isoalkanes, < 2% aromatics	918-167-1
C9-14 Aliphatics (<=2% aromatic)	Hydrocarbons, C11-C13, isoalkanes, < 2% aromatics	920-901-0
C9-14 Aliphatics (<=2% aromatic)	Hydrocarbons, C10-C13, n-alkanes, < 2% aromatics	929-018-5
C9-14 Aliphatics (<=2% aromatic)	Hydrocarbons, C11-C14, n-alkanes, < 2% aromatics	924-803-9

C9-14 Aliphatics (<=2% aromatic)	Hydrocarbons, C9-C11, cyclics, < 2% aromatics	925-894-8
C9-14 Aliphatics (<=2% aromatic)	Decane	204-686-4
C9-14 Aliphatics (<=2% aromatic)	Undecane	214-300-6
	Dodecane	203-967-9
C9-14 Aliphatics (<=2% aromatic)	Tridecane	211-093-4
	Tetradecane	211-096-0
C9-14 Aliphatics (<=2% aromatic)	Isododecane	297-629-8
C9-14 Aliphatics (<=2% aromatic)	Hydrocarbons, C10-C14, n-alkanes, isoalkanes, <2% aromatic	920-274-3
C9-14 Aliphatics (<=2% aromatic)	Hydrocarbons, C11-C12, isoalkanes, cyclics, <2% aromatics	931-121-5
C14-20 Aliphatics (<=2% aromatic)	Hydrocarbons, C13-C18, n-alkanes, isoalkanes, cyclics, < 2% aromatics	928-253-0
C14-20 Aliphatics (<=2% aromatic)	Hydrocarbons, C14-C18, n-alkanes, isoalkanes, cyclics, < 2% aromatics	927-632-8
C14-20 Aliphatics (<=2% aromatic)	Hydrocarbons, C16-C20, n-alkanes, isoalkanes, cyclics, < 2% aromatics	919-029-3

C14-20 Aliphatics (<=2% aromatic)	Hydrocarbons, C13-C16, isoalkanes, cyclics, < 2% aromatics	918-973-3
C14-20 Aliphatics (<=2% aromatic)	Hydrocarbons, C14-C19, isoalkanes, cyclics, < 2% aromatics	920-114-2
C14-20 Aliphatics (<=2% aromatic)	Hydrocarbons, C14-C17, n-alkanes, < 2% aromatics	917-828-1
C14-20 Aliphatics (<=2% aromatic)	Hydrocarbons, C14-C20, n-alkanes, < 2% aromatics	923-583-1
C14-20 Aliphatics (<=2% aromatic)	Pentadecane	211-098-1
C14-20 Aliphatics (<=2% aromatic)	Hexadecane (n-Hexadecane)	Pre-registration 208-878-9 Reg. 2018
C14-20 Aliphatics (<=2% aromatic)	Hexadecane (iso-hexadecane)	297-628-2
C14-20 Aliphatics (<=2% aromatic)	Heptadecane	Pre-registration 211-108-4 Reg. 2018
C14-20 Aliphatics (<=2% aromatic)	Octadecane	Pre-registration 209-790-3 Reg. 2018
C14-20 Aliphatics (<=2% aromatic)	Icosane (isoicosane)	Pre-registration 297-627-7 Reg. 2013
C14-20 Aliphatics (<=2% aromatic)	Icosane (n-icosane)	204-018-1
C14-20 Aliphatics (<=2% aromatic)	Hydrocarbons, C14-C20, n-alkanes, isoalkanes, <2% aromatics	931-265-9