

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 for hydrocarbon solvents 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).
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- 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.

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 and o-xylene, will be described as "mixture of m-xylene and o-xylene".

² RIP3.10 chapter 4

³ RIP 3.10 subchapter 4.2.2

⁴ RIP 3.10 chapter 4.3

And as last the category which includes the substances related to this naming convention,

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

Substances which can not be specified by one chemical name of the constituents, as not all the constituents can be identified or they may be specified but with a lack of specificity due to the variability of the exact composition.

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: the split into 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. The PINA structure can be determined by GC/MS and/or 2D GC or any equivalent test method.
- 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.

Notes:

-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.

- Products consisting out of components which are blended or mixed outside the production process or the petroleum refineries are not considered as substances, but as preparations. As such these products do not need to be registered, as long as the blending components are registered.

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-C11 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.

Example 1:

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	35	40	11	3

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 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 and C12 makes 96%. 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-C12**".

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-C12, **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-C12, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)".

Final name for REACH registration:

Hydrocarbons, C9-C12, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)

Other Examples:

Example 2:

I have a white spirit with similar PINA split but and a carbon number range which fits into above range, but is narrower?

Carbon number	C8	C9	C10	C11	C12	C13
Amount in %	0	17	66	17	0	0

Naming should be Hydrocarbons, C9-C11, n-alkanes, isoalkanes, cyclics, aromatics (2-25%), but since more than 80% of the composition and carbon range fits in the existing name of example 1 and as long as classification and labeling is identical, the substance can be categorized as being similar and named: Hydrocarbons, C9-C12, n-alkanes,

isoalkanes, cyclics, aromatics (2-25%)". This is to prevent that too many different substance names are created for products which are in fact very similar in composition and have identical classification and labelling.

Example 3:

I have again a white spirit with similar PINA split, but a heavier carbon number range:

Carbon number	C8	C9	C10	C11	C12	C13
Amount in %	0	0	10	20	60	10

However this product is classified as non-flammable, while the two white spirits of the previous examples are classified inflammable (R10).

Although more than 80% of the composition fits in the naming of example 1, this product will be categorized with another substance name, to prevent that it should receive an unnecessary labeling for flammability, inherent to the substance name. A new substance name should be chosen: Hydrocarbons, **C10-C13**, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)

Example 4:

I have a dearomatized white spirit with a PINA split of 25% n-paraffins, 45% isoparaffins, 29.5% cyclics and 0.5% aromatics.

The carbon number range is:

Carbon number	C8	C9	C10	C11	C12	C13
Amount in %	3	14	35	40	8	0

Although the carbon number range fits into the name of example one, this product is part of a different HPV category due to its aromatic content which is below the cut off value of 2% and as such this product will also have a different classification. A new substance name should be given, indicating the different HPV category:

Hydrocarbons, C9-C11, n-alkanes, isoalkanes, cyclics, **<2% aromatics**

Example 5:

I have a synthetic hydrocarbon solvent with no n-paraffins or cyclics, but 99% isoparaffins and 1% aromatics.

The carbon number range is:

Carbon number	C8	C9	C10	C11	C12	C13
Amount in %	0	6	35	35	22	2

Due to its low aromatic content the product belongs to the HPV category, C9-14 Aliphatics (<=2% aromatic), as is the product in example 4. However the specific high isoparaffins purity characterizes this product and determines it to specific enduses. The absence of cyclics and n-paraffins can, or will possibly, lead to a different classification or labeling. To avoid that high purity synthetic substances will be mixed with more general petroleum distillates, a specific naming should be given, here: Hydrocarbons, C10-C12, isoalkanes, <2% aromatics.

Example 6:

Technical hexane contains mainly n-paraffins (n-hexane 60%), but also some C6 isoparaffins (iso-hexanes 20%) and some C6 cyclics (cyclohexanes 20%). Aromatic content is below 0.01 %.

Since all components are C6's the product belongs to the HPV category of the C6 aliphatics and its name will start with Hydrocarbons, C6,.

Since the isoparaffins and cyclics are both present in an amount of more than 10%, they need to appear in the naming. The aromatics are below the cut off value and should, according to the HPV category name, not be mentioned.

n-Hexane however triggers a classification R48 when present in an amount over the 5%.

Therefore the n-hexane should appear in the naming, mentioning the cut off value.

(Above 80% of n-hexane, product may be named as a pure substance) :

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

Attachment 3:

Example of info required in a pre-registration document:

To be completed.

Attachment 4:

Defined substances per HydroCarbon Solvents Consortium category:

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

C9 Aromatics
Hydrocarbons, C9, aromatics
C10-12 Aromatics
Hydrocarbons, C10, aromatics, >1% naphthalene
Hydrocarbons, C10, aromatics, <1% naphthalene
Hydrocarbons, C10-C13, aromatics, <1% naphthalene
Hydrocarbons, C10-C13, aromatics, >1% naphthalene
C9-14 Aliphatics (2-25% aromatics)
Hydrocarbons, C9-C10, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)
Hydrocarbons, C10-C13, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)
Hydrocarbons, C8-12, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)
Hydrocarbons, C9-C12, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)
Hydrocarbons, C11-C14, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)
Hydrocarbons, C10-C14: isoalkanes, cyclics, aromatics(2-25%)
C14-20 Aliphatics (2-30% aromatic)
Hydrocarbons, C14-C18, n-alkanes, isoalkanes, cyclics, aromatics (2-30 %)
Hydrocarbons, C16-C20, n-alkanes, isoalkanes, cyclics, aromatics (2-30 %)
C5 Aliphatics
Normal-Pentane
ISO-Pentane
Cyclopentane
Hydrocarbons, C5, n-alkanes, isoalkanes
C6 Aliphatics
Normal-Hexane
Iso-Hexane
Cyclohexane
Hydrocarbons, C6, n-alkanes, isoalkanes, cyclics, n-hexane rich
Hydrocarbons, C5-C7, n-alkanes, isoalkanes, < 5% n-hexane
Hydrocarbons, C6-C7, isoalkanes, cyclics, < 5% n-hexane

Methylcyclopentane
Hydrocarbons, C5-C7, n-alkanes, isoalkanes, n-hexane rich
C7-9 Aliphatics
Hydrocarbons, C7, n-alkanes, isoalkanes, cyclics
Hydrocarbons, C6-C7, n-alkanes, isoalkanes, cyclics, > 5% n-hexane
Hydrocarbons, C6-C7, n-alkanes, isoalkanes, cyclics, < 5% n-hexane
Hydrocarbons, C7-C9, n-alkanes, isoalkanes, cyclics
Hydrocarbons, C6-C10, n-alkanes, isoalkanes, > 5% n-hexane
Hydrocarbons, C7-C9, isoalkanes
Hydrocarbons, C7-C8, cyclics
Normal-Heptane
Iso-Heptane
Normal-Octane
Iso-Octane
Nonane
C9-14 Aliphatics (<=2% aromatic)
Hydrocarbons, C9-C11, n-alkanes, isoalkanes, cyclics, < 2% aromatics
Hydrocarbons, C9-C10, n-alkanes, isoalkanes, cyclics, < 2% aromatics
Hydrocarbons, C9-C11, isoalkanes, cyclics, < 2% aromatics
Hydrocarbons, C10-C13, n-alkanes, isoalkanes, cyclics, < 2% aromatics
Hydrocarbons, C10-C13, isoalkanes, cyclics, < 2% aromatics
Hydrocarbons, C11-C14, n-alkanes, isoalkanes, cyclics, < 2% aromatics
Hydrocarbons, C13-C15, n-alkanes, isoalkanes, cyclics, < 2% aromatics
Hydrocarbons, C12-C15, n-alkanes, isoalkanes, cyclics, < 2% aromatics
Hydrocarbons, C11-C14, isoalkanes, cyclics, < 2% aromatics
Hydrocarbons, C10-C12, isoalkanes, < 2% aromatics
Hydrocarbons, C11-C12, isoalkanes, < 2% aromatics
Hydrocarbons, C11-C13, isoalkanes, < 2% aromatics
Hydrocarbons, C10-C13, n-alkanes, < 2% aromatics
Hydrocarbons, C11-C14, n-alkanes, < 2% aromatics
Hydrocarbons, C9-C11, cyclics, < 2% aromatics
Decane
Undecane
Dodecane
Tridecane
Tetradecane
Isododecane
Hydrocarbons, C10-C13, Isoalkanes <2% aromatics
Hydrocarbons, C10-C14, n-alkanes, <2% aromatics
Hydrocarbons, C10-C14, n-alkanes, isoalkanes, <2% aromatic
Hydrocarbons, C12-C15, n-alkanes, isoalkanes, cyclics, < 2% aromatics

C14-20 Aliphatics (<=2% aromatic)
Hydrocarbons, C13-C18, n-alkanes, isoalkanes, cyclics, < 2% aromatics
Hydrocarbons, C14-C18, n-alkanes, isoalkanes, cyclics, < 2% aromatics
Hydrocarbons, C16-C20, n-alkanes, isoalkanes, cyclics, < 2% aromatics
Hydrocarbons, C16-C20, n-alkanes, isoalkanes, < 2% aromatics
Hydrocarbons, C13-C16, isoalkanes, cyclics, < 2% aromatics
Hydrocarbons, C14-C19, isoalkanes, cyclics, < 2% aromatics
Hydrocarbons, C14-C17, n-alkanes, < 2% aromatics
Hydrocarbons, C14-C20, n-alkanes, < 2% aromatics
Pentadecane
Hexadecane
Heptadecane
Octadecane
Nonadecane
Icosane
Hydrocarbons, C14-C20, n-alkanes, isoalkanes, <2% aromatics