

Substance identification and naming convention for hydrocarbon solvents

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Substance identification and naming convention for hydrocarbon solvents

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 / 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.

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

¹ Guidance for identification and naming of substances under REACH and CLP § 4.3.1.2

- 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 Guidance for identification and naming of substances under REACH and CLP.
- 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 way in which hydrocarbon solvents were identified for purposes of data submission to meet the requirements of the OECD HPV (High Production Volume) initiative (see attachment 4).

Three types of substances have been defined by REACH in the ECHA guidance²:

1) Mono-constituent substances, which consist off more than 80% 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 concentrations between 10 and 80%.⁴

The composition must be known and more than one constituent is relevant for the identification of the substance. The chemical composition of the substance is predictable, as typical values and ranges.

These substances will be described as specified in ECHA guidance as a reaction mass of the main constituents of the substance as such.

Example given in the guidance: Xylene, consisting of more than 10% of m-xylene and o-xylene, p-xylene is considered as impurity (<10%), will be described as "Reaction mass of m-xylene and o-xylene".

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

² Guidance for identification and naming of substances under REACH and CLP § 4

³ Guidance for identification and naming of substances under REACH and CLP § 4.2.1

⁴ Guidance for identification and naming of substances under REACH and CLP § 4.2.2

⁵ Guidance for identification and naming of substances under REACH and CLP § 4.3

A number of hydrocarbon solvents meet the criteria for UVCB substances as the number of discrete chemical constituents is relatively large and the composition of all discrete chemical components is variable and cannot always be identified.

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 all 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 toxicological properties or classifications** will be mentioned, using the classification cut-off as an indication level (according to Annex VI of EU regulation EC/1272/2008 as known as CLP).

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 determine if they fit into one of the existing HSPA naming categories. If the substance fit within the existing categories, the producer can join the HSPA consortium and benefit from read across for data on the corresponding category.

Attachment 1

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

An example of the 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:

Components	amount
Normal paraffins	25 %
Isoparaffins	25 %
Cycloparaffins	49.6 %
Aromatics	0.4 %

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

In the ECHA guidance for identification of substances, 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 cycloparaffins with carbon number of C9, C10 and C11 have been provided.

Difference depending on the chosen naming description:

	EINECS number	HSPA naming 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	Indicated as < 2%
Hazard classification	Hazards could include R11, R20, R45, R46, R48, R63 R38, R65, R66, R67 and/or R51/53 (depending on the presence of various components at varying levels)	R10, R65, R66 (components requiring other classifications are not present in that substance)

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% (1ppm). 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 cycloparaffinic) 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 rules described in ECHA guidance for identification and naming of substances under REACH and CLP. The components identified by hydrocarbon type and carbon number range must represent at least 80% of the total composition and individual components at levels above 10% must be mentioned. Individual components at level below 10% are not included in the naming of the substance unless they trigger a health or environmental classification.

In this case we do not know all the constituents for each carbon number range, as the C8, C12 and C13 hydrocarbon components represent less than 10% of the total substance and following the ECHA guidance it's not necessary to mention them. The remaining components represent more than 80% of the composition: i.e the sum of C9, C10 & C11 is 92%. Since the composition of each isomer of each of the C9, C10 and C11 hydrocarbons is variable 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 ECHA guidance for identification and naming of substances rules, 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 be mentioned in the substance name. So the name must include n-alkanes, isoalkanes, cyclics and aromatics.

Regular white spirit falls within the category of substances identified as "C9-C14 Aliphatics (2-25% aromatics)" and was identified in that way as part of the OECD HPV process. 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 because, if benzene is present at a level of or above 0.1%, the substance has to be classified as carcinogenic. As the level of benzene is below this regulatory cut-off point the substance is not classified on the basis of benzene content and there is 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 rich".

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

Attachment 3

Defined substances per REACH registration Dossier

You can find below the list of the hydrocarbon substances REACH registered, grouped by HPV category:

Category 1 : C9 Aromatics	
Substance name	EC Number
Hydrocarbons, C9, aromatics	918-668-5
Hydrocarbons, C9-C10, aromatics >1% naphthalene	946-365-8

Category 2 : C9-12 Aromatics	
Substance name	EC Number
Hydrocarbons, C10, aromatics, <1% naphthalene	918-811-1
Hydrocarbons, C10, aromatics, >1% naphthalene	919-284-0
Hydrocarbons, C10-C13, aromatics, <1% naphthalene	922-153-0
Hydrocarbons, C10-C13, aromatics, >1% naphthalene	926-273-4

Category 3 : C9-14 Aliphatics (2-25% Aromatics)	
Substance name	EC Number
Hydrocarbons, C10-C13, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)	919-164-8
Hydrocarbons, C11-C14, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)	925-653-7
Hydrocarbons, C12-C16, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)	920-008-6
Hydrocarbons, C9-C10, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)	927-344-2
Hydrocarbons, C9-C12, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)	919-446-0

Category 4: C14-20 Aliphatics (2-30% aromatic)	
Substance name	EC Number
Hydrocarbons, C14-C18, n-alkanes, isoalkanes, cyclics, aromatics (2-30 %)	920-360-0
Hydrocarbons, C16-C20, n-alkanes, isoalkanes, cyclics, aromatics (2-30 %)	919-006-8

Category 5: C5 Aliphatics	
Substance name	EC Number
Cyclopentane	206-016-6
Hydrocarbons, C5, n-alkanes, isoalkanes	921-577-3
Iso-Pentane (2-methylbutane)	201-142-8
Normal-Pentane	203-692-4

Category 6: C6 Aliphatics	
Substance name	EC Number
2,2 Dimethyl-butane	200-906-8
2,3 Dimethyl-butane	201-193-6
2-Methyl-pentane	639-864-4
Hydrocarbons, C5-C7, n-alkanes, isoalkanes, <5% n-hexane	922-114-8
Hydrocarbons, C5-C7, n-alkanes, isoalkanes, n-hexane rich	930-397-4
Hydrocarbons, C6, isoalkanes, <5% n-hexane	931-254-9

Category 6: C6 Aliphatics	
Substance name	EC Number
Hydrocarbons, C6, n-alkanes, isoalkanes, cyclics, n-hexane rich	925-292-5
Hydrocarbons, C6-C7, isoalkanes, cyclics, <5% n-hexane	926-605-8
n-Hexane	203-777-6

Category 7: C7-9 Aliphatics	
Substance name	EC Number
2,2,3 Triméthyl-butane	207-346-3
2,2,4-triméthylpentane	208-759-1
Hydrocarbons, C6-C10 (even numbered), n-alkanes, isoalkanes, >5% n-hexane	701-352-4
Hydrocarbons, C6-C7, n-alkanes, isoalkanes, cyclics, <5% n-hexane	921-024-6
Hydrocarbons, C6-C7, n-alkanes, isoalkanes, cyclics, >5% n-hexane	924-168-8
Hydrocarbons, C7, n-alkanes, isoalkanes, cyclics	927-510-4
Hydrocarbons, C7-C8, cyclics	927-033-1
Hydrocarbons, C7-C8, isoalkanes, <2% aromatics	947-588-3
Hydrocarbons, C7-C8, n-alkanes	922-214-1
Hydrocarbons, C7-C9, isoalkanes	921-728-3
Hydrocarbons, C7-C9, n-alkanes, isoalkanes, cyclics	920-750-0
Hydrocarbons, C8-C9, isoalkanes	932-020-9
Iso-Heptane	250-610-8
Isooctane (UVCB)	247-861-0
Nonane	203-913-4
Normal-Heptane	205-563-8
Normal-Octane	203-892-1

Category 8: C9-14 Aliphatics (<=2% aromatic)	
Substance name	EC Number
Alkanes, C10-13-iso	271-366-9
Alkanes, C12-14 iso-	271-369-5
C09 C11 N-Alkanes < 2% Aromatics	927-807-9
Decane	204-686-4
Dodecane	203-967-9
Hydrocarbons, C10-C12, isoalkanes, <2% aromatics	923-037-2
Hydrocarbons, C10-C12, n-alkanes, <2% aromatics	926-527-4
Hydrocarbons, C10-C13, isoalkanes, cyclics, <2% aromatics	918-317-6
Hydrocarbons, C10-C13, n-alkanes, <2% aromatics	929-018-5
Hydrocarbons, C10-C13, n-alkanes, isoalkanes, <2% aromatics	940-726-3
Hydrocarbons, C10-C13, n-alkanes, isoalkanes, cyclics, <2% aromatics	918-481-9
Hydrocarbons, C10-C14 (even numbered), n-alkanes, isoalkanes, <2% aromatics	920-274-3
Hydrocarbons, C11-C12, isoalkanes, <2% aromatics	918-167-1
Hydrocarbons, C11-C12, n-alkanes, <2% aromatics	928-282-9
Hydrocarbons, C11-C13 (odd number), n-alkanes, <2% aromatics	942-924-5
Hydrocarbons, C11-C13, isoalkanes, <2% aromatics	920-901-0
Hydrocarbons, C11-C14, isoalkanes, cyclics, <2% aromatics	927-285-2
Hydrocarbons, C11-C14, n-alkanes, <2% aromatics	924-803-9
Hydrocarbons, C11-C14, n-alkanes, isoalkanes, <2% aromatics	701-280-3
Hydrocarbons, C11-C14, n-alkanes, isoalkanes, cyclics, <2% aromatics	926-141-6
Hydrocarbons, C11-C16, n-alkanes, isoalkanes, <2% aromatics	942-085-5
Hydrocarbons, C12-C14, isoalkanes, cyclics, <2% aromatics	701-198-8

Category 8: C9-14 Aliphatics (<=2% aromatic)	
Substance name	EC Number
Hydrocarbons, C12-C15, n-alkanes, isoalkanes, <2% aromatics	940-727-9
Hydrocarbons, C12-C15, n-alkanes, isoalkanes, cyclics, <2% aromatics	920-107-4
Hydrocarbons, C12-C16, isoalkanes, cyclics, < 2% aromatics	927-676-8
Hydrocarbons, C13-C14, n-alkanes, <2% aromatics	939-519-0
Hydrocarbons, C13-C15, n-alkanes, isoalkanes, cyclics, <2% aromatics	917-488-4
Hydrocarbons, C4, 1,3-butadiene-free polymd, triisobutylene fraction, hydrogenated	297-629-8
Hydrocarbons, C8-C11, n-alkanes, isoalkanes, <2% aromatics	940-733-1
Hydrocarbons, C9-C10, n-alkanes, isoalkanes, cyclics, <2% aromatics	927-241-2
Hydrocarbons, C9-C11, cyclics, <2% aromatics	925-894-8
Hydrocarbons, C9-C11, isoalkanes, cyclics, <2% aromatics	920-134-1
Hydrocarbons, C9-C11, n-alkanes, isoalkanes, <2% aromatics	941-718-2
Hydrocarbons, C9-C11, n-alkanes, isoalkanes, cyclics, <2% aromatics	919-857-5
Hydrocarbons, C9-C12, n-alkanes, isoalkanes, <2% aromatics	940-725-8
Isododecane (2,2,4,6,6-pentamethylheptane)	236-757-0
Tetradecane	211-096-0
Tridecane	211-093-4
Undecane	214-300-6

Category 9: C14-20 Aliphatics (<=2% aromatic)	
Substance name	EC Number
Hexadecane	208-878-9
Hydrocarbons, C13-C16, Isoalkanes, <2% aromatics	946-885-5
Hydrocarbons, C13-C16, isoalkanes, cyclics, <2% aromatics	918-973-3
Hydrocarbons, C13-C18, n-alkanes, isoalkanes, cyclics, <2% aromatics	928-253-0
Hydrocarbons, C14-C15, n-alkanes, <2% aromatics	928-868-4
Hydrocarbons, C14-C16, n-alkanes, <2% aromatics	921-535-4
Hydrocarbons, C14-C16, n-alkanes, isoalkanes, <2% aromatics	940-728-4
Hydrocarbons, C14-C17, isoalkanes, cyclics, <2% aromatics	939-601-6
Hydrocarbons, C14-C17, n-alkanes, <2% aromatics	917-828-1
Hydrocarbons, C14-C18, n-alkanes, isoalkanes, cyclics, <2% aromatics	927-632-8
Hydrocarbons, C14-C19, isoalkanes, cyclics, <2% aromatics	920-114-2
Hydrocarbons, C14-C20 (even numbered), n-alkanes, isoalkanes, <2% aromatics	700-976-4
Hydrocarbons, C14-C20, n-alkanes, <2% aromatics	923-583-1
Hydrocarbons, C15-C16, n-alkanes, <2% aromatics	943-046-5
Hydrocarbons, C15-C19, n-alkanes, isoalkanes, <2% aromatics	940-730-5
Hydrocarbons, C16-C18, Isoalkanes, <2% aromatics	948-766-3
Hydrocarbons, C16-C20, n-alkanes, isoalkanes, cyclics, <2% aromatics	919-029-3
Hydrocarbons, C17-C19, n-alkanes, <2% aromatics	937-158-3
Hydrocarbons, C4, 1,3-butadiene-free, polymd., tetraisobutylene fraction, hydrogenated	297-628-2
Icosane	204-018-1
Isoeicosane (Hydrocarbons, C4, 1,3-butadiene-free, polymd., pentaisobutylene fraction, hydrogenated)	297-627-7
Isohexadecane (2,2,4,4,6,8,8 heptamethylnonane)	224-506-8
N-Heptadecane	211-108-4
Octadecane	209-790-3
Pentadecane	211-098-1

Attachment 4

Substances identified but not falling in one of the predefined HPV categories

Hydrocarbons, C10-C17, n-alkanes, isoalkanes, cyclics, aromatics (10-25 %)

Note: Check if 80% of composition fits into C9-14 or C14-20.

*If not read across may be possible with category C9-14 Aliphatics (2-25% aromatics)
or C14-20 Aliphatics (2-30% aromatics)*

Hydrocarbons, C12-C16, n-alkanes, isoalkanes, cyclics, <2% aromatics

Hydrocarbons, C12-C16, isoalkanes, cyclics, <2% aromatics

*Note: Check if 80% composition fits into C9-13 Aliphatics (=< 2% aromatics) or
C14-20 Aliphatics (=< 2% aromatics)*

If not read across may be possible with one of these two categories.

Hydrocarbons, C13-C20, n-alkanes, isoalkanes, cyclics, aromatics (40-60 %)

Note: Read across may be possible with category C14-20 Aliphatics (2-30% aromatics)