concawe

GUIDANCE ON REPORTING ANALYTICAL INFORMATION FOR PETROLEUM UVCB SUBSTANCES IN REACH REGISTRATION DOSSIERS

VERSION 2.0

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Contents

1. Disclaimer

The information in this document has been prepared in good faith, based on information and guidance currently available. Neither CONCAWE nor any of its Member Companies can accept any liability arising from the use of the information included in this document. It is to be relied upon at the user's own risk.

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2. Purpose of this document

This document provides guidance regarding how to obtain the analytical information for the identification of Petroleum Substances and how to present it in the REACH registration dossier (IUCLID Sections 1.2 and 1.4). Most Petroleum Substances are **UVCB**s (Substances of **U**nknown or **V**ariable composition, **C**omplex reaction products or **B**iological materials) and are addressed in this guidance; this guidance does not address mono-constituent substances such as Sulfur.

It must be emphasised that, in spite of intensive discussions between CONCAWE and ECHA, no consensus has been reached yet over the appropriate set of information necessary to identify Petroleum UVCB Substances. In particular, ECHA has stated that additional analytical and spectral data may be requested from registrants of Petroleum UVCB Substances should the dossier be selected for a compliance check. Although the discussions with ECHA will continue, this document only reflects current CONCAWE views.

In April 2014 ECHA has started sending information letters to registrants in the context of an automated IT screening of substance identification data in registration dossiers (the Substance Identity – SID – screening campaign). Additional information on ECHA screening activities can be found at ECHA's website (http://www.echa.europa.eu/en/web/guest/support/how-to-improve-your-dossier/it-screening-campaigns-on-dossiers). Together with the information letters, registrants have received a Technical Annex containing more information on the 10 issues addressed in the SID screening campaign, as well as the recommended next steps (http://www.echa.europa.eu/documents/10162/13552/technical_annex_sid_screening_en.pdf). On 30 April 2014 ECHA held a webinar to explain how to address substance identity issues that have been identified as an outcome of the SID screening campaign; the presentations can be found at the following link (http://www.echa.europa.eu/web/guest/view-article/-/journal_content/title/substance-identity-issues-covered-in-the-screening-campaign).

This document provides CONCAWE's recommendations to address the SID issues relevant for Petroleum UVCB Substances and will make reference to the relevant sections of ECHA's Technical Annex.

3. Background

CONCAWE has prepared IUCLID5 files for the joint registration of Petroleum Substances, applying a category approach. When appropriate, specific information for each category is provided in this document.

Reflecting the fact that the Petroleum UVCB Substances are derived originally from crude oil, their composition is typically not only variable but also very complex. For

example, several hundred different hydrocarbon structures may be present in naphtha streams, whilst this number rises to an estimated many thousands in heavy streams.

Individual CAS/EINECS number definitions have been developed to describe the products of different refining processes and these typically describe Petroleum Substances in terms of feedstock source, refining process, predominant carbon number range and approximate boiling point range.

General information requirements and certain key principles of substance identification are defined in Annex VI of the REACH Regulation (EC) No 1907/2006. The ECHA "Guidance for identification and naming of substances under REACH and CLP" (http://echa.europa.eu/documents/10162/13643/substance_id_en.pdf) includes provisions for UVCB substances, plus more specific information for Petroleum Substances. Additional information on CONCAWE's approach can be found in the CONCAWE Report 7/12 "REACH – Analytical characterisation of petroleum UVCB substances", which can be freely downloaded from CONCAWE website (https://www.concawe.eu).

4. Information on substance identification in the IUCLID5 registration dossiers

Information on substance identification related to composition and analytical techniques is required in two places in the IUCLID5 dossiers, in Section 1.2 – Composition and in Section 1.4 – Analytical Information. CONCAWE recommends to registrants of Petroleum UVCB Substances to include the following information.

4.1. Section 1.2 – Composition

Concentration ranges (i.e. "Minimum" and "Maximum" values) should be provided for all constituents (and additives where relevant) for which the registrant provides information, together with "Typical" values. Since these data have to be registration-specific, CONCAWE is not able to offer "standard" concentration ranges and therefore this information needs to be provided by each registrant.

The following options are suggested to derive reasonable estimates of the variability of the substance's composition:

- Historic data
- Several *ad-hoc* analyses
- Statistical estimations / Modelling
- Expert judgement

The following fields in IUCLID5 Section 1.2 should be filled. Note that the registration files provided by CONCAWE already include some pre-filled content for each Petroleum UVCB Substance, as specified below.

4.1.1. Composition Header

- The field "Name" provided by CONCAWE contains the name of the registered substance itself (as described in IUCLID5 Section 1.1) and can be edited by each registrant if needed.
- The field "Brief description" should be completed by each registrant to provide a description of the procedure used to derive the concentration ranges and the typical values.

- The “Degree of purity” should be reported as 100 “% (w/w)” (as provided by CONCAWE) since UVCBs do not contain impurities by definition.

4.1.2. Constituents

At least one constituent should be reported (see Issue type 3 in ECHA’s Technical Annex). The registered substance itself (as described in IUCLID5 Section 1.1) should not be included as a constituent.

Individual constituents present at ≥ 10% w/w and constituents (“markers”) relevant for hazard classification or PBT assessment (independently of their concentration) should be reported and individually identified via a link to a Reference Substance containing appropriate substance identifiers (EC, CAS, IUPAC, etc). Appendix 3 lists for each category the constituents relevant for hazard classification or PBT assessment.

Hydrocarbon Classes should be reported and identified via a link to a Reference Substance containing a generic description of their chemical nature (see Appendix 1 for the Hydrocarbon classes provided by the recommended analytical methods). For the Naphthas category, the concentrations for the Hydrocarbon Classes (Paraffins, Iso-paraffins, Olefins, Naphthenics, and Aromatics) should be reported net of any constituents individually reported (e.g. those present at ≥ 10% w/w or being classification markers).

Unknown constituents (e.g. unassigned GC peaks) should be reported and identified via a link to the Reference Substance “Unknown Constituents”. It is recommended to only use this when analyses have unassigned peaks.

For each constituent reported, the following fields should be filled (see IUCLID5 screenshot under Issue type 1 in ECHA’s Technical Annex).

- The “Reference substance” should contain a link to the appropriate Reference Substance.
- The “Typical concentration” value should be reported as “ca.” [Typical value] “% (w/w)” and must be within the concentration range specified below (see Issue type 2 in ECHA’s Technical Annex).
- The “Concentration range” should be reported as “>=” [Minimum value] “<=” [Maximum value] “% (w/w)”.

A standard set of constituents is provided by CONCAWE, containing all required data except the concentration values. These constituents cover, for each category, the information provided by the recommended analytical methods (see Appendixes 1 and 2) and also the constituents relevant for classification or PBT assessment (see Appendix 3).

For certain categories (e.g. Naphthas), additional constituents may be required to identify individual hydrocarbons present at ≥ 10% w/w. Note that the corresponding Reference Substances are not provided by CONCAWE, and therefore registrants are advised to download the necessary Reference Substances from the IUCLID website (http://iuclid.eu/index.php?fuseaction=home.downloadsubstances); see Issue type 10 in ECHA’s Technical Annex for more information.

4.1.3. Impurities

Petroleum UVCB Substances do not contain impurities by definition. UVCBs are single substances containing constituents which account for 100% of the total composition.

4.1.4. Additives

Petroleum products may contain a number of chemical additives that can be added at various stages after the manufacturing process and/or in the supply chain:

- **Stabilising additives (stabilisers)** to maintain product integrity, are present at concentrations too low (typically a few ppm to a few hundred ppm) to need to be considered in the substance identity. Stabilisers will need to be identified in IUCLID5 Section 1.2 of the registration dossier provided that the information is available to the registrant (see IUCLID5 screenshot under Issue type 9 in ECHA's Technical Annex).
- **Performance/Other Additives** – additives and blending components added to enhance the performance of the product or to meet regulatory requirements (which may be present at concentrations of a few hundreds ppm to 10% or more) or other purposes are not considered to be part of the substance. Performance or other additives in petroleum products have to be registered separately as components of mixtures.

4.2. Section 1.4 – Analytical information

The analytical data including the description of the analytical methods and the actual results of analysis shall be reported in IUCLID section 1.4.

The following fields in IUCLID5 Section 1.4 should be filled, except in REACH registration dossiers for intermediates under Strictly Controlled Conditions. See IUCLID5 screenshot under Issue type 8 in ECHA's Technical Annex.

4.2.1. Analytical information

- The field "Analytical information and spectral data" should contain a waiving statement for the analytical and/or spectral methods not applied (delete entries as appropriate): "**GC, LC, IR, UV, NMR, MS are not necessary in accordance with Note 1 in Annex VI of the REACH Regulation. Any additional information on molecular structure does not contribute to substance identification further to the information provided below.**"
- The field "Optical activity" should contain a waiving statement like "**Not relevant**" or "**Not applicable**" since this is not applicable to Petroleum UVCB Substances.

4.2.2. Results of analysis

The following entries should be provided to describe the analytical methods applied (see Issue type 8 in ECHA's Technical Annex).

- Boiling point range and carbon number range; note that these data will not be part of IUCLID5 Section 1.2 and, when applicable, should be consistent with the EINECS definition of the registered substance.
- Analytical method(s) used to determine the composition of the substance (see Appendixes 1 and 2). The results reported here should lie within the concentration ranges reported in IUCLID5 Section 1.2. Chromatographic and spectral data should be provided in an interpreted form, i.e. with peaks assigned to components or groups of components and, if feasible, be quantified in "% w/w".
- When appropriate (see Appendix 1), Viscosity; note that these data will not be part of IUCLID5 Section 1.2 and should be consistent with the classification of the registered substance as described in the registrant's MSDS.

For each entry, the following fields should be filled (see IUCLID5 screenshot under Issue type 8 in ECHA's Technical Annex).

- The field "Analysis type" should contain a name describing the type of analysis (e.g. "Simulated distillation", "Gas chromatography", etc).
- The field "Tested substance" should contain the description of the material subject to analysis (normally the registered substance itself).
- The field "Method used" should contain the reference to the analytical method used. Registrants applying modified standard test methods should provide a description of the test conditions according to ECHA's recommendations in the "Guidance for identification and naming of substances under REACH and CLP".
- An attachment should be provided containing the analytical results, annotated and quantified.
- The field "Remarks" should contain any additional information.

Appendix 1 Recommended methods for analytical information on petroleum UVCB substances

The test methods listed below are only indicative. CONCAWE is aware that many registrants apply modified standard test methods. However, unless these modified test methods have been published the analytical data would have to be supplemented by a description of the test conditions, according to ECHA recommendations in the "Guidance for identification and naming of substances under REACH".

List of analytical methods for each category of Petroleum UVCB substances

The following abbreviations have been used: NMR for Nuclear Magnetic Resonance, GC for Gas Chromatography, LC for Liquid Chromatography, HPLC for High-Performance Liquid Chromatography, TLC-FID for Thin Layer Chromatography and Flame Ionisation Detection, IBP for Initial Boiling Point and FBP for Final Boiling Point.

The methods used should be suitable for the type of product being analysed; in some cases the lighter and/or heavier members of a category may require different analytical methods. See Appendix 2 for the scope of the analytical methods.

Legend:		
	=	means: two or more methods are equivalent; they provide the same information on the composition of a substance
	or	means: two or more methods are alternative options; they provide similar, but not necessarily the same information
	% w/w	means: % weight on weight; note that mol % obtained by NMR spectroscopy will have to be transformed into % w/w

Category	**Standard Analytical Methods**				**Content of IUCLID5 Section 1.2 (see chapter 4.1)**	**Content of IUCLID5 Section 1.4 (see chapter 4.2)**
	Boiling point and Carbon number range by Physical [P] or Simulated [S] Distillation	**Individual Hydrocarbons or Hydrocarbon Classes**	**Viscosity (marker for Aspiration Hazard)**	**DMSO extract (marker for Carcinogenicity)**		
Low Boiling Point Naphthas (Gasolines)	[P] EN3405=ASTMD86 [S] ASTMD3710 or ASTMD7096	Detailed Hydrocarbon Analysis DHA (GC): ASTMD5134 or ASTMD6729 or ASTMD6730 Reformulyser PIONA (GC): EN22854=ASTMD6839			• classification markers (see Appendix 3) • constituents present at ≥10% w/w • % w/w of each identified hydrocarbon class (net of any constituents reported individually) ▪ paraffins ▪ iso-paraffins ▪ olefins ▪ naphthenics ▪ aromatics	• Boiling point range • Carbon number range • GC trace
Kerosines	[P] EN3405=ASTMD86 [S] EN3924=IP406=ASTMD2887	IP436=ASTMD6379 (HPLC) or EN12916=IP391 (HPLC)			• % w/w of hydrocarbon classes ▪ IP436: mono- and di-aromatic hydrocarbons, or ▪ IP391: mono-, di- and tri+ aromatic hydrocarbons	• Boiling point range • Carbon number range • HPLC trace

Category	Standard Analytical Methods				Content of IUCLID5 Section 1.2 (see chapter 4.1)	Content of IUCLID5 Section 1.4 (see chapter 4.2)
	Boiling point and Carbon number range by Physical [P] or Simulated [S] Distillation	Individual Hydrocarbons or Hydrocarbon Classes	Viscosity (marker for Aspiration Hazard)	DMSO extract (marker for Carcinogenicity)		
MK1 diesel fuel	[P] EN3405=ASTMD86 [S] EN3924=IP406=ASTM D2887	IP436=ASTMD6379 (HPLC) or EN12916=IP391 or IP548=ASTMD6591 (HPLC) or ASTMD2007 (LC)			• % w/w of hydrocarbon classes ▪ IP436: mono- and di-aromatic hydrocarbons, or ▪ IP391/IP548: mono-, di- and tri+ aromatic hydrocarbons, or ▪ LC: saturated, aromatic and polar hydrocarbons	• Boiling point range • Carbon number range • HPLC trace or LC report
Straight-run Gas Oils	[P] EN3405=ASTMD86 [S] EN3924=IP406=ASTM D2887	EN12916=IP391 or IP548=ASTMD6591 (HPLC) or ASTMD2007 (LC)			• % w/w of hydrocarbon classes ▪ HPLC: mono-, di- and tri+ aromatic hydrocarbons, or ▪ LC: saturated, aromatic and polar hydrocarbons	• Boiling point range • Carbon number range • HPLC trace or LC report
Cracked Gas Oils	[P] EN3405=ASTMD86 [S] EN3924=IP406=ASTM D2887	EN12916=IP391 or IP548=ASTMD6591 (HPLC) or ASTMD2007 (LC)			• % w/w of hydrocarbon classes ▪ HPLC: mono-, di- and tri+ aromatic hydrocarbons, or ▪ LC: saturated, aromatic and polar hydrocarbons	• Boiling point range • Carbon number range • HPLC trace or LC report
Vacuum Gas Oils, Hydrocracked Gas Oils & Distillate Fuels	[P] EN3405=ASTMD86 [S] EN3924=IP406=ASTM D2887	EN12916=IP391 or IP548=ASTMD6591 (HPLC) or ASTMD2007 (LC)	EN3104		• % w/w of hydrocarbon classes ▪ HPLC: mono-, di- and tri+ aromatic hydrocarbons, or ▪ LC: saturated, aromatic and polar hydrocarbons	• Boiling point range • Carbon number range • HPLC trace or LC report • Viscosity
Other Gas Oils	[P] EN3405=ASTMD86 [S] EN3924=IP406=ASTM D2887	EN12916=IP391 or IP548=ASTMD6591 (HPLC) or ASTMD2007 (LC)	EN3104		• % w/w of hydrocarbon classes ▪ HPLC: mono-, di- and tri+ aromatic hydrocarbons, or ▪ LC: saturated, aromatic and polar hydrocarbons	• Boiling point range • Carbon number range • HPLC trace or LC report • Viscosity
Heavy Fuel Oil Components	[S] EN15199-1=IP480 or EN15199-2=IP507	EN12916=IP391 (HPLC) or ASTMD2007 (LC) or IP392 or ASTMD5292 (NMR)	EN3104		• % w/w of hydrocarbon classes ▪ HPLC: mono-, di- and tri+ aromatic hydrocarbons, or ▪ LC: saturated, aromatic and polar hydrocarbons ▪ NMR: aromatic and non-aromatic carbon	• Boiling point range • Carbon number range • HPLC trace or LC report or NMR spectrum • Viscosity
Unrefined / Acid Treated Oils	[S] EN15199-1=IP480 or EN15199-2=IP507	ASTMD2007 (LC) or IP392 or ASTMD5292 (NMR)	EN3104		• % w/w of hydrocarbon classes ▪ LC: saturated, aromatic and polar hydrocarbons ▪ NMR: aromatic and non-aromatic carbon	• Boiling point range • Carbon number range • LC report or NMR spectrum • Viscosity

Category	Standard Analytical Methods				Content of IUCLID5 Section 1.2 (see chapter 4.1)	Content of IUCLID5 Section 1.4 (see chapter 4.2)
	Boiling point and Carbon number range by Physical [P] or Simulated [S] Distillation	Individual Hydrocarbons or Hydrocarbon Classes	Viscosity (marker for Aspiration Hazard)	DMSO extract (marker for Carcinogenicity)		
Other Lubricant Base Oils	[S] EN15199-1=IP480 or EN15199-2=IP507	IP368 or ASTMD7419 (HPLC) or ASTMD2007 (LC) or IP392 or ASTMD5292 (NMR)	EN3104	IP346	• % w/w of hydrocarbon classes ▪ HPLC: saturated and aromatic hydrocarbons, or ▪ LC: saturated, aromatic and polar hydrocarbons ▪ NMR: aromatic and non-aromatic carbon • % w/w DMSO extract	• Boiling point range • Carbon number range • HPLC trace or LC report • Viscosity • DMSO extract
Highly Refined Base Oils	[S] EN15199-1=IP480 or EN15199-2=IP507	IP368 or ASTMD7419 (HPLC) or ASTMD2007 (LC) or IP392 or ASTMD5292 (NMR)	EN3104		• % w/w of hydrocarbon classes ▪ HPLC: saturated and aromatic hydrocarbons, or ▪ LC: saturated, aromatic and polar hydrocarbons ▪ NMR: aromatic and non-aromatic carbon	• Boiling point range • Carbon number range • HPLC trace or LC report or NMR spectrum • Viscosity
Foots Oils	[S] EN15199-1=IP480 or EN15199-2=IP507	ASTMD2007 (LC) or IP392 or ASTMD5292 (NMR)	EN3104	IP346	• % w/w of hydrocarbon classes ▪ LC: saturated, aromatic and polar hydrocarbons ▪ NMR: aromatic and non-aromatic carbon • % w/w DMSO extract	• Boiling point range • Carbon number range • LC report or NMR spectrum • Viscosity • DMSO extract
Paraffin and Hydrocarbon Waxes	[S] EN15199-1=IP480 or EN15199-2=IP507	ASTMD2007 (LC) or IP392 or ASTMD5292 (NMR)			• % w/w of hydrocarbon classes ▪ LC: saturated, aromatic and polar hydrocarbons ▪ NMR: aromatic and non-aromatic carbon	• Boiling point range • Carbon number range • LC report or NMR spectrum
Slack Wax	[S] EN15199-1=IP480 or EN15199-2=IP507	ASTMD2007 (LC) or IP392 or ASTMD5292 (NMR)		IP346 (in the base oil from which the substance was produced)	• % w/w of hydrocarbon classes ▪ LC: saturated, aromatic and polar hydrocarbons ▪ NMR: aromatic and non-aromatic carbon • % w/w DMSO extract	• Boiling point range • Carbon number range • LC report or NMR spectrum • DMSO extract
Petrolatum	[S] EN15199-1=IP480 or EN15199-2=IP507	ASTMD7419 (HPLC) or IP392 or ASTMD5292 (NMR)		IP346 (in the base oil from which the substance was produced)	• % w/w of hydrocarbon classes ▪ HPLC: saturated and aromatic hydrocarbons, or ▪ NMR: aromatic and non-aromatic carbon • % w/w DMSO extract	• Boiling point range • Carbon number range • HPLC trace or NMR spectrum • DMSO extract

Category	Standard Analytical Methods				Content of IUCLID5 Section 1.2 (see chapter 4.1)	Content of IUCLID5 Section 1.4 (see chapter 4.2)
	Boiling point and Carbon number range by Physical [P] or Simulated [S] Distillation	Individual Hydrocarbons or Hydrocarbon Classes	Viscosity (marker for Aspiration Hazard)	DMSO extract (marker for Carcinogenicity)		
Untreated Distillate Aromatic Extracts	[S] EN15199-1=IP480 or EN15199-2=IP507	ASTMD2007 (LC) or IP392 or ASTMD5292 (NMR)	EN3104		• % w/w of hydrocarbon classes ▪ LC: saturated, aromatic and polar hydrocarbons ▪ NMR: aromatic and non-aromatic carbon	• Boiling point range • Carbon number range • LC report or NMR spectrum • Viscosity
Treated Distillate Aromatic Extracts	[S] EN15199-1=IP480 Or EN15199-2=IP507	ASTM2007 (LC) or IP392 or ASTMD5292 (NMR)	EN3104	IP346	• % w/w of hydrocarbon classes ▪ LC: saturated, aromatic and polar hydrocarbons ▪ NMR: aromatic and non-aromatic carbon • % w/w DMSO extract	• Boiling point range • Carbon number range • LC report or NMR spectrum • Viscosity • DMSO extract
Residual Aromatic Extracts	[S] EN15199-1=IP480 or EN15199-2=IP507	ASTMD2007 (LC) or IP392 or ASTMD5292 (NMR)			• % w/w of hydrocarbon classes ▪ LC: saturated, aromatic and polar hydrocarbons ▪ NMR: aromatic and non-aromatic carbon	• Boiling point range • Carbon number range • LC report or NMR spectrum
Bitumen	[S] EN15199-1=IP480 or EN15199-2=IP507	ASTMD2007 (LC) or IP469 (TLC-FID)			• % w/w of hydrocarbon classes ▪ LC: saturated, aromatic and polar hydrocarbons, asphaltenes, or ▪ TLC-FID: saturated, aromatic and polar hydrocarbons, asphaltenes	• Boiling point range • Carbon number range • LC report or TLC-FID trace

Appendix 2 Industry Standard Analytical Methods for Identification of Petroleum Products

Method	Title	Analyte(s)	Scope	Comments
PHYSICAL DISTILLATION [P]				
EN3405= ASTMD86	*Petroleum products — Determination of distillation characteristics at atmospheric pressure*	specific temperatures representing 0.5% (IBP), 5%, 10%, 20% ... 95% and 99.5% (FBP) sample recovery	Naphthas, Kerosines, MK1, Gas Oils IBP>0°C and FBP<400°C	Carbon number range estimated by comparison with the boiling points of n-alkanes
SIMULATED DISTILLATION BY GC [S]				
ASTMD3710	*Boiling Range Distribution of Gasoline and Gasoline Fractions by Gas Chromatography*	specific temperatures representing 0.5% (IBP), 5%, 10%, 20% ... 95% and 99.5% (FBP) sample recovery	Naphthas FBP<260°C	Carbon number range estimated by comparison with the boiling points of n-alkanes
ASTMD7096	*Determination of the Boiling Range Distribution of Gasoline by Wide-Bore Capillary Gas Chromatography*	specific temperatures representing 0.5% (IBP), 5%, 10%, 20% ... 95% and 99.5% (FBP) sample recovery	Naphthas FBP<280°C	Carbon number range estimated by comparison with the boiling points of n-alkanes
EN3924= IP406= ASTMD2887	*Boiling Range Distribution of Petroleum Fractions by Gas Chromatography*	specific temperatures representing 0.5% (IBP), 5%, 10%, 20% ... 95% and 99.5% (FBP) sample recovery	Kerosines, MK1, Gas Oils FBP<538°C	Carbon number range estimated by comparison with the boiling points of n-alkanes
EN15199-1= IP480	*Petroleum products - Determination of boiling range distribution by gas chromatography method - Part 1: Middle distillates and lubricating base oils*	specific temperatures representing 0.5% (IBP), 5%, 10%, 20% ... 95% and 99.5% (FBP) sample recovery	Heavier than Gas Oils IBP>100°C and FBP<750°C	Carbon number range estimated by comparison with the boiling points of n-alkanes
EN15199-2= IP507	*Petroleum products - Determination of boiling range distribution by gas chromatography method - Part 2: Heavy distillates and residual fuels*	specific temperatures representing 0.5% (IBP), 5%, 10%, 20% ... sample recovery and final elution temperature (FBP)	Heavier than Gas Oils IBP>100°C and FBP>750°C	Carbon number range estimated by comparison with the boiling points of n-alkanes
DETAILED HYDROCARBON ANALYSIS BY GC [DHA]				
ASTMD5134	*Detailed Analysis of Petroleum Naphthas through n-Nonane by Capillary Gas Chromatography*	hydrocarbon components (including n-hexane and BTEX) components eluting after n-nonane determined as a single group	Naphthas <2% olefins components <151°C	the results should be used to determine the Carbon number range
ASTMD6729	*Determination of Individual Components in Spark Ignition Engine Fuels by 100 Metre Capillary High Resolution Gas Chromatography*	hydrocarbon components (including n-hexane and BTEX) and oxygenates (MeOH, EtOH, BuOH, MTBE, ETBE, TAME)	Naphthas <25% olefins components <225°C	the results should be used to determine the Carbon number range
ASTMD6730	*Determination of Individual Components in Spark Ignition Engine Fuels by 100–Metre Capillary (with Precolumn) High-Resolution Gas Chromatography*	hydrocarbon components (including n-hexane and BTEX) and oxygenates (MeOH, EtOH, BuOH, MTBE, ETBE, TAME)	Naphthas <25% olefins components <225°C	the results should be used to determine the Carbon number range

Method	Title	Analyte(s)	Scope	Comments
SELECTIVE HYDROCARBON ANALYSIS BY MULTIDIMENSIONAL GC [REFORMULYSER PIONA]				
EN22854= ASTMD6839	*Liquid petroleum products — Determination of hydrocarbon types and oxygenates in automotive-motor gasoline — Multidimensional gas chromatography method*	saturated, aromatic and olefinic hydrocarbons, benzene and oxygenates	Naphthas 1.5-30% olefins, <50% aromatics, <2% benzene and 0.8-15% oxygenates FBP<215°C	
HYDROCARBON CLASS ANALYSIS BY HPLC				
IP436= ASTMD6379	*Determination of aromatic hydrocarbon types in aviation fuels and petroleum distillates – High performance liquid chromatography method with refractive index detection*	mono- and di-aromatic hydrocarbons	Kerosines and MK1 0-75% mono-aromatics and 0-25% di-aromatics boiling point range 50-300°C	
EN12916= IP391	*Petroleum products - Determination of aromatic hydrocarbon types in middle distillates – High performance liquid chromatography method with refractive index detection*	mono-, di- and tri+ aromatic hydrocarbons	Kerosines, MK1 and Gas Oils boiling point range 150-400°C	without backflush
IP548= ASTMD6591	*Determination of aromatic hydrocarbon types in middle distillates – High performance liquid chromatography method with refractive index detection*	mono-, di- and tri+ aromatic hydrocarbons	MK1 and Gas Oils boiling point range 150-400°C	with backflush
IP368	*Determination of hydrocarbon types in lubricating oil basestocks – Preparative high performance liquid chromatography method*	saturated and aromatic hydrocarbons	Base Oils IBP>270°C	gravimetric measurement of analytes with backflush
ASTMD7419	*Determination of Total Aromatics and Total Saturates in Lube Basestocks by High Performance Liquid Chromatography (HPLC) with Refractive Index Detection*	saturated and aromatic hydrocarbons	Base Oils and Petrolatums 0.2-46% aromatics	with backflush
HYDROCARBON CLASS ANALYSIS BY LC				
ASTMD2007	*Characteristic Groups in Rubber Extender and Processing Oils and Other Petroleum-Derived Oils by the Clay-Gel Absorption Chromatographic Method*	saturated, aromatic and polar hydrocarbons asphaltenes (if the pentane insoluble content is ≥0.1)	Heavier than Naphthas IBP>260°C and FBP>400°C	HPLC methods are preferred since they give a breakdown of aromatics by number of rings
HYDROCARBON CLASS ANALYSIS BY TLC-FID				
IP469	*Determination of saturated, aromatic and polar compounds in petroleum products by thin layer chromatography and flame ionisation detection*	saturated, aromatic and polar hydrocarbons asphaltenes	Bitumen IBP>300°C	

Method	Title	Analyte(s)	Scope	Comments
HYDROCARBON CLASS ANALYSIS BY SPECTROSCOPY				
IP392	*Determination of aromatic hydrogen and carbon content – High resolution nuclear magnetic resonance spectroscopy method*	mole percent aromatic hydrogen and aromatic carbon	Heavier than Gas Oils except Bitumen	
ASTMD5292	*Aromatic Carbon Contents of Hydrocarbon Oils by High Resolution Nuclear Magnetic Resonance Spectroscopy*	mole percent aromatic hydrogen and aromatic carbon	Heavier than Gas Oils except Bitumen	
VISCOSITY MEASUREMENT				
EN3104	*Petroleum products - Transparent and opaque liquids - Determination of kinematic viscosity and calculation of dynamic viscosity*	kinematic viscosity	liquid petroleum products	dynamic viscosity calculated from kinematic viscosity and density
HYDROCARBON CLASS ANALYSIS BY SOLVENT EXTRACTION				
IP346	*Determination of polycyclic aromatics in unused lubricating base oils and asphaltene free petroleum fractions – Dimethyl sulfoxide extraction refractive index method*	polycyclic aromatic hydrocarbons (three or more fused rings)	1-15% polycyclic aromatics IBP>300°C	gravimetric measurement of analyte correlation between IP346 results and *in-vitro* mutagenicity (Ames Test)

Appendix 3 Constituents relevant to hazard classification and PBT assessment of Petroleum UVCB Substances

Category/Standalone substances	Constituents relevant to hazard classification (threshold concentration % w/w indicated in brackets)		Constituents relevant to PBT assessment (when present at concentrations greater than 0.1 % w/w)
	Dangerous Substances Directive (DSD)	Classification, Labelling & Packaging Regulation (CLP)	
Low Boiling Point Naphthas (Gasolines) [1]	Benzene (0.1 %) Toluene (5 %) n-Hexane (5 %)	Benzene (0.1 %) Toluene (3 %) n-Hexane (3 %)	None
Kerosines and MK1 Diesel Fuel [1]	None	None	None
Straight-run Gas Oils [2]	None	None	None
Vacuum Gas Oils, Hydrocracked Gas Oils & Distillate Fuels [2]	None	None	None
Cracked Gas Oils [2]	None	None	None
Other Gas Oils [2, 3]	None	None	None
Heavy Fuel Oil Components	None	None	None
Unrefined / Acid Treated Oils	None	None	None
Highly Refined Base Oils [2]	None	None	None
Lubricant Base Oils [2, 4]	DMSO extract	DMSO extract	None
Untreated Aromatic Extracts	None	None	None
Treated Distillate Aromatic Extracts [4]	DMSO extract	DMSO extract	None
Residual Aromatic Extracts [5]	None	None	None
Slack Wax [3]	None [6]	None [6]	None
Paraffin and Hydrocarbon Waxes	None	None	None
Petrolatum [3]	None [6]	None [6]	None
Foots oils [4]	DMSO extract	DMSO extract	None
Bitumen	None	None	None

Footnotes in the table above:

[1] For all members of this category, the overall viscosity of the substance measured at 40 ºC is less than 7 cSt (DSD) and less than 20.5 cSt (CLP), therefore resulting in classification for aspiration hazard.

[2] In addition to chemical constituents, for this category the overall viscosity of the substance also needs to be considered for hazard classification when less than 7 cSt for DSD and less than 20.5 cSt for CLP, always measured at 40 ºC.

[3] Substances in this category have to be classified as Carcinogenic unless the full refining history is known and it can be shown that the substance from which it is produced is not a carcinogen.

[4] In addition to chemical constituents, for this category the DMSO extract (IP346 method) of the substance also needs to be considered for hazard classification when greater than 3 % w/w.

[5] Substances in this category have to be classified as Carcinogenic unless the Mutagenicity Index is <0.4.

[6] IP346 determined in the base oil from which the substance was produced.