AN INTERNATIONALLY RECOGNIZED NOMENCLATURE SYSTEM FOR PETROLEUM ADDITIVES

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1. BACKGROUND:

1.1 ATC

The ATC (Additives Technical Committee) is the Technical Committee of Petroleum Additive Manufacturers in Europe. It represents a research-intensive industry, generating performance products, i.e. products designed to deliver a particular chemical behaviour rather than to provide a specific chemical composition.

1.2 History and Regulatory background

It was noted by J. A. Henry [1] as recently as 1998 that complex chemical names "are of little value to medical personnel or other health specialists, who generally have only limited knowledge of chemical nomenclature. Simpler names which are familiar to those handling the product or advising on its safe use are therefore more effective in expressing essential safety messages or conveying information for the benefit of employers, employees, emergency services and first aid personnel, and also in general for the medical profession." These views have been expressed in broadly similar terms on a number of occasions over the past few years [2,3,4].

The EU's Dangerous Substances Directive [5] (Article 23) indicates that, where chemical names are required on labels, they should be given in one of the designations given in Annex I. If the substance is not yet listed in Annex I, the name must be given using an "internationally recognized designation." Annex I does not only use systematic names and the term internationally recognized designation, is not defined in any EU directive. However, several such systems are widely known, e.g. CAS (Chemical Abstracts Services of the American Chemical Society), IUPAC (International Union of Pure and Applied Chemistry), Colour Index, Pesticides, SDA (Soap and Detergents Association) ATC and INCI (International Nomenclature of Cosmetic Ingredients).

These systems vary greatly in their simplicity and the extent to which they disclose precise chemistry. The ATC nomenclature system, described in this Document, is designed to facilitate disclosure of sufficient information to ensure protection of the environment, and of the health and safety of users of the products, whilst protecting the reasonable and legitimate intellectual property rights of manufacturers, within the letter and spirit of the law. It has been used successfully by Petroleum Additive Manufacturers to protect the exact chemical identity of a substance for the following purposes:

1. Supporting confidentiality claims with respect to new chemical notifications in Canada and the publication of Safety Data Sheets under Hazardous Materials Information Review Commission (HMIRC) guidelines in this country.

2. Submitting confidential Pre-Manufacturing or Pre-Marketing Notices (PMNs) in the US, EU, and most other regulatory jurisdictions.

3. Supporting submissions for confidentiality requests to EU Member State Competant Authorities under Article 15 of the current Dangerous Preparations Directive[6].

4. Supporting water-hazard classifications (Wassergefährdungsklasse or WGK) submitted to the Office of Commission for the Evaluation of Substances Hazardous to Waters (KBwS) at Umweltbundesamt (UBA) in Germany.

Finally, it may be mentioned that the data collection exercises currently being managed jointly by government and the chemical industry throughout the world use ATC nomenclature.

2. PROTECTION OF INTELLECTUAL PROPERTY:

2.1 Industry Concerns:

The ATC is concerned about the protection of the intellectual property of its member companies, particularly the precise chemical names of many of its proprietary petroleum additives. ATC agrees that sufficient information about the identity of chemicals must always be made available to permit the safe use and handling of these additives. Very precise information about the chemical identity of chemicals is always made available to medical professionals and Competent Authorities as needed, with the proviso that such information be kept confidential.

The Committee maintains the view that indiscriminate and uniformed public disclosure of the precise compositional details of additives in formulations is of little practical benefit to its customers. This is due to the fact that there is a basic lack of public expertise in interpreting complex chemical names and thereby a critical lack of the knowledge necessary to protect man and the environment in a meaningful and efficient manner. Industry also believes that any unilateral requirement to reveal the specific chemical names of substances in their products will negatively impact the market success of these products and critically reduce the resource necessary to research and generate less hazardous products for the future. In this context, ATC believes that neither the IUPAC nor the CAS systems offer an appropriate methodology for developing and disclosing the names of chemicals in its products.

2.2 Comparison of Nomenclature Systems:

Petroleum additives are generally difficult to name in the IUPAC or CAS systems. They are usually complex mixtures of closely related chemical species and are named after the major component(s) or functional groups. They also typically contain significant levels of diluent oil or other solvents to facilitate processing and product handling. This diluent may for example be a severely refined mineral oil, a light hydrocarbon, an oxygenated solvent, etc. For these reasons, petroleum additives manufacturers, suppliers, and their customers prefer the use of the more generalized and still functionally descriptive ATC nomenclature system which focuses increasing attention upon the main structural and physiological features which comprise those chemicals placed on the market.

This system, first formalized in the early 1980s, results in the derivation of generic chemical names which are easily recognized internationally and hence have added

special communicative value when used to label products and their corresponding safety data sheets. These names are typically shorter than CAS or IUPAC names and they immediately signal to a health professional any physiologically active chemical groups present. The following table illustrates how the nomenclature derived from two more complex systems compares with that suggested by the ATC system. These three chemicals are some of the least complex substances used by the industry.

ATC Name	IUPAC Name	CAS Name
Zinc dialkyl dithiophosphate	Zinc bis[O,O-bis-(1-methylethyl) phosphorodithioato-S,S']-, (T-4)	Phosphorodithioic acid, di-isopropyl ester, zinc salt.
Magnesium long- chain alkaryl sulphonate	Benzene, 2,4-di-(2-methyl-C11-15) sulphonic acid, magnesium salt	Benzene sulphonic acid, C_{12}-C_{16} alkyl derivatives, magnesium salts
Polyalkenyl succinimide	2,5 Furandione, dihydro-, 3-(polybutenyl) derivatives, reaction products with tetraethylene pentamine	Amines, polyethylenepoly, reaction products with polybutenyl succinic anhydride derivatives

3. KEY CRITERIA FOR A NOMENCLATURE SYSTEM:

A nomenclature system intended for broad general use must satisfy certain criteria for acceptability. It must be:

- Logical, consistent and informative without requiring esoteric interpretive chemical skills,
- Readily and logically extendable to similar but new products,
- Indicative regarding structural constitution associated with any potential physiological activity,
- Informative enough to establish a consistent basis for safe use and handling practices.

4. BASIC CONCEPTS OF THE ATC NOMENCLATURE SYSTEM:

4.1 Major Structural Moieties:

Chemical additives can typically be described in generic terms or descriptors once one has evaluated the molecular structures and other specialized features present. For example, these chemicals often contain:

- Metals in ionic form
- Hydrocarbon based fragments, cyclic, acyclic, branched or linear, aromatic.
- Functional groups that connect desired moieties together into a single molecular structure.

For complex chemicals, these descriptors must be assembled in a logical sequence, bearing in mind the need for the name to provide essential technical and toxicological clues to their behaviour. In this way, the ATC nomenclature system meets the key requirements set out in section 3 above.

4.2 Metal/Substrate Linkage:

Any metal present must be logically linked with its generic functional substrate, such as sulphonate, phenate, salicylate, phosphate, etc.

4.3 Hydrocarbyl Type Descriptors:

Hydrocarbyl type descriptors may comprise but are not restricted to those listed in the following table:

Descriptor	**Meaning**	**Examples**
Alkyl	C_1 to C_{10}, saturated straight or branched chain	Butyl, octyl, isopropyl, 2-ethylhexyl
Long-chain alkyl	Saturated straight or branched chain ≥C_{11}	Dodecyl, 3-propylundecyl, eicosyl
Long-chain alkaryl	Saturated straight or branched chain ≥C_{11} + aryl group	Dodecylphenyl, octadecylphenyl
Aryl	Aromatic hydrocarbon group	Phenyl, naphthyl
Alkaryl	C_1 to C_{10} Alkyl-aryl group	Ethylphenyl, decylphenyl
Alkenyl	C_1 to C_{10} group containing at least one double bond	Octenyl, methyloctenyl
Long-chain alkenyl	≥C_{11} group containing at least one double bond	Dodecenyl, octadecenyl
Akylene	C_1 to C_{10} disubstituted alkane	Ethylenedi… (as in ethylene diamine)
Polyolefin	Polymerized alkene	Polyisobutene or polypropylene
Terpene	Member of the terpenes group	Alpha-pinene
Hydrocarbyl	Ill-defined hydrocarbon group	Mixed straight and branched chain alkanes and alkenes

Note: A more specific carbon number range, or other information, would be added if this might have toxicological significance. In cases where technological knowledge might be disclosed in this way, the manufacturer may request that the user accept this information under confidential cover.

4.4 Active Group Descriptors:

Examples of active group descriptors will be found in the following list:

Acid, acyl	Phenate [a, b]
Acrylate, acrylo, acrylic	Phosphate
Alcohol, alcoxy, oxy, aryloxy	Phosphite

Alkyleneamine	Phosphonate, phosphonite, phosphinic
Amide, amido	Phosphorosulphide
Amine, amino, ammonium	Phosphorus oxyacid/ester [c]
Anhydride	Polyacid, polyester
Borate, borate ester	Polyalkylene glycol
Boric acid derivative, borated	Polyalkylenepolyamine
Carbonate, carbamate	Polyamine, polyamide
Carboxylic acid, carboxy, carboxylate	Polyether, polyoxyalky
Chlorosulphide	Polyfumarate
Dithiophosphate, dithionate	Polyol, polyoxy, polyoxyalkylene
Ester, esterified	Polysiloxane, polysilane
Ether, ethoxylated	Salicylate [a], salicylic, salicyl
Hydroxyl, hydroxylated, hydroxy	Salt (inorganic only)
Imidazole, imidazolene, imidazolenone	Silicate
Imide, di-imide	Succinic, succinimide, succinate ester, succinyl
Ketone, carbonyl, keto, oxo	Sulphide, thiol, thioether
Maleated	Sulphonate [a]
Mercaptan, mercaptyl	Sulphurized, polysulphurized
Methacrylate, methacryl	Thiazine, thiadiazole, thioamide, thiourea
Naphthenate	Thiocarbamate, dithiocarbamate
Nitrate, nitrite, nitric, nitrile	Triazole, triazine, triazolenone
Nitro, nitrilo	Urea, urethane
Peroxide, peroxy	

In addition, one could create any number of additional unspecified combinations of the above descriptors to more completely describe all of the functional aspects of a chemical substance in generic terms. One need not be limited by those options presented herein. The over arching principal governing the proper use of this system is that virtually all functional chemical moieties described in the chemical literature today are more commonly referred to using generic descriptor for the sake of simplicity without loss of clarity or meaning.

Notes:

a. For some product groups, e.g. sulphonate, phenate and salicylate detergents, it may be necessary to distinguish between ‘overbased’ and ‘non-overbased’ (or ‘neutral’) products. ‘Overbased’ means that the product contains additional metal carbonate in micellar form.

b. Also known as phenoxylate or phenoxide.

c. Only used in cases where it is not clear whether the group is an oxyacid or an ester.

5. EXAMPLES OF ATC NOMENCLATURE: Principles of the System.

The principal aim of the system is to help maintain as much consistency in chemical group names as possible when composing generic names for chemicals. Whilst a suggested ordering of the principal functional words and phrases has been promoted historically, such conventions are not intended to be restrictive and should always take clear account the meaningful transmission of critical structural details. The following examples may help illustrate this approach.

If the chemical is the result of a reaction between an acid and a base, it is helpful to initially focus on that aspect of the chemical structure. For example, “calcium phenate” would indicate the reaction product of a base (Calcium Hydroxide) and Phenol (the acid species). If the phenol involved bears certain alkyl substituents, these can be reflected in the modifier e.g. alkyl phenol. Should the alkylphenol in this example be sulphurized, additional modifiers can be employed resulting in the term “calcium alkylphenate, sulphurized”. An alternative description, such as “Calcium Alkylphenate Sulphide” might be confusing, insofar as one might conclude that this chemical also contains the elements of Calcium Sulphide. In the example above, the term “sulphurized” conveys a reaction step that involves the chemical insertion of sulphur to some degree as opposed to the incorporation of a potentially hazardous sulphide.

Working backwards from the ATC name itself, one can similarly understand the intended meaning of the following generic chemical name: “Magnesium Alkaryl Sulphonate”. From the outset, it is clear that this substance is a magnesium salt of the sulphonic acid class of chemicals. More specifically, this salt is a derivative of an aryl sulphonic acid. The aryl group, which bears the sulphonic acid moiety, also comprises alkyl substituents. There would therefore be little ambiguity between this substance and an alkyl sulphonate.

When applied to the generic naming of neutral chemicals, the same general thinking applies. Focus is placed upon the principal chemical feature of the substance being considered. Take for example, succinimides. The term “alkenylsuccinimide” is a description derived from the chemical root, succinic acid. The implication is that this acid moiety links together an unspecified alkenyl group with an amine capable of forming an imide. A polyisobutenyl succinimide, molybdenum sulphide would satisfactorily describe a succinimide that has been used to form a chemical complex with a specific metal sulphide.

Using the concepts of the ATC nomenclature system as set out above, the following are some examples of internationally recognized names for current major petroleum additives in common use today. ATC Document No. 49 shows many of the chemical structures referred to below and is a useful companion guide for developing additional chemical names similar to those referred to below. It can be seen that this system of nomenclature conveys important information about the physical and chemical properties of complex chemical substances without revealing specific details about unique raw materials and proprietary manufacturing processes.

6. SPECIFIC EXAMPLES OF ATC NOMENCLATURE:

6.1 Zinc and Other Oxyphosphorus Additives:

Zinc alkaryl dithiophosphate

Zinc alkyl dithiophosphate

6.2 Other Metal-Based Additives:

Barium long-chain alkaryl sulphonate

Calcium long-chain alkaryl sulphonate

Calcium long-chain alkyl phenate

Calcium long-chain alkyl phenate, sulphurized

Calcium long-chain alkyl salicylate

Magnesium long-chain alkaryl sulphonate

Magnesium long-chain alkyl phenate, sulphurized

Magnesium long-chain alkyl salicylate

Sodium long-chain alkaryl sulphonate

6.3 Nitrogen-containing Additives:

Alkyl ammonium dithiophosphate

Alkyl dithio thiadiazole

Alkyl nitrate

Long-chain alkaryl polyether amidoamine

Long-chain alkylpolyamide amine

Polyamine

Polyalkyl amino phenol

Polyamino polyamide

Polyether amide

Polyether amine

Polyolefin amide alkyleneamine

Polyolefin amide alkyleneamine borate

Polyolefin amine, polyolefin polyamine

Polyolefin succinimide

Polyolefin succinimide, borated

Polyolefin sucinimide, molybdenum sulphide complex

6.4 Sulphides, Phosphorosulphides and Halogen-containing Additives:

Polyolefin phosphorosulphide

Polyalkyl polysulfide

Polyolefin sulphide

Long-chain alkyl acid/ester sulphides

Long-chain alkenyl thioester

6.5 Polymeric Additives:

Alkaryl polyether

Alkyl ester copolymer

Aryl polyolefin

Hydrocarbyl polymer

Long-chain alkaryl polyether

Olefin/alkylester copolymer

Polyacrylate ester

Polyalkylene glycol

Poly long-chain alkyl methacrylate

Polyether

Polyol

Polyolefin

Polyolefin ester

6.6 Other Additives:

Alkylphenol, hindered alkylphenol

Branched alkylbenzene, linear alkylbenzene

Long-chain alkane, long chain α-olefin

Long-chain alkaryl sulphonic acid

Long-chain alkyl carboxylic acid

Long-chain alkyl salicylic acid

Long-chain alkylester

Severely refined virgin mineral oil

7. REFERENCES:

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