

AN INTERNATIONALLY RECOGNIZED
NOMENCLATURE SYSTEM FOR
PETROLEUM ADDITIVES

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INTRODUCTION:

It was noted by J. A. Henry¹ 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 Directive⁵ (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, ATC and US Environmental Protection Agency. These systems vary greatly in their simplicity and the extent to which they disclose precise chemistry. The ATC nomenclature system, described in this Document, sets out to achieve a balance between protecting the health and safety rights of those handling or using a product and protecting the reasonable and legitimate intellectual property rights of manufacturers, always within the meaning of the law. 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:

1.1 Industry Concerns: The Technical Committee of Petroleum Additive Manufacturers in Europe (ATC) represents a research-intensive industry generating performance products, i.e. products designed to perform a particular task rather than to provide or include a specific chemical entity. It is therefore vitally concerned about the protection of the intellectual property of its member companies, particularly the precise chemical nature of petroleum additives. ATC believes that sufficient information must always be made available to permit the safe use and handling of these additives. It also believes that public disclosure of the precise compositional details of additives is not in the interests of its customers, because lack of protection will reduce the incentive to generate better products. In this context, ATC believes that neither IUPAC nor CAS offers an appropriate system of nomenclature for its products.

1.2 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). They also typically contain significant levels of diluent to facilitate product handling. This diluent may be a severely refined mineral oil or a hydrocarbon or oxygenated solvent. For these reasons, the petroleum additives industry and its customers use a more generalized nomenclature based on the main structural components, i.e. metal, hydrocarbon type and active (usually organic) group. This system, first formalized in the early 1980s, results in names that are recognized internationally by users and manufacturers and hence have special value for user labelling and data sheets. They are shorter than CAS or IUPAC names and they immediately indicate to a health professional any physiologically active groupings present. The following examples illustrate how the nomenclature systems compare:

| ATC Name | IUPAC Name | CAS Name |
|---|--|---|
| Zinc alkyl dithiophosphate | Zinc, di-isopropyl dithiophosphate | Phosphorodithioic acid, 0,0 bis (1-methylethyl) ester, zinc salt |
| Magnesium long-chain alkaryl sulphonate | Magnesium di-(C ₁₂ -C ₁₆ alkyl) benzene sulphonate | Benzene sulphonic acid, C ₁₂ -C ₁₆ alkyl derivatives, magnesium salts |
| Alkenyl succinimide | Polyisobutenyl succinic anhydride/ tetraethylene pentamine condensate | 2,5-Furandione, dihydro monopolybutenyl derivatives, reaction products with tetraethylene pentamine |

3. KEY CRITERIA FOR A NOMENCLATURE SYSTEM: A nomenclature system for general use must satisfy certain criteria. It must:

- * be logical, consistent and informative without being cumbersome or requiring esoteric chemical skills;
- * be able to describe current products and be readily and logically extendable to cover new products and types of products;
- * provide information on chemical constitution indicative of potential physiological activity; and
- * provide sufficient information to represent a sound basis for establishing safe use and handling practices.

4. BASIC CONCEPTS OF THE ATC NOMENCLATURE SYSTEM:

4.1 Major Structural Moieties: The molecule is divided into major structural moieties, e.g.:

- * metal
- * hydrocarbon type descriptor(s)
- * active group descriptor(s)

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

4.2 Metal/Substrate Linkage: Each metal must be linked to a specific substrate, such as sulphonate or phenate.

4.3 Hydrocarbon Type Descriptors: Examples of hydrocarbon type descriptors are given in the following table:

| Descriptor | Meaning | Examples |
|-------------------|---|---|
| Alkyl | C ₁ to C ₁₀ , saturated straight or branched | Butyl or isopropyl |
| Long-chain alkyl | C ₁₁ To C ₄₀ saturated straight or branched chain | Dodecyl or 3-propyl undecyl |
| Aryl | Aromatic hydrocarbon group | Phenyl |
| Alkaryl | Alkyl-aryl group | Ethylphenyl |
| Alkenyl | C ₁ to C ₁₀ group containing at least one double bond | Octenyl or methyloctenyl |
| Akylene | C ₁ to C ₁₀ disubstituted alkane | Ethylenedi... (as in ethylene diamine) |
| Polyolefin | Polymerized alkene | Polybutene or polyisobutylene |
| 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 know-how 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 | phenyl |
| acrylate | phenate ^{a, b} |
| alcohol | phosphite |
| alkyleneamine | phosphate |
| amine | phosphonate |
| amide | phosphorosulphide |
| anhydride | phosphorus oxyacid/ester ^c |
| borate | polyacid |
| boric acid derivative | polyalkylene glycol |
| carbonate | polyalkylenepolyamine |
| carboxylic acid | polyamine |
| chlorosulphide | polyether |
| copolymer | polyol |
| dithiophosphate | polysiloxane |
| ester | salicylate ^a |
| ester polymer | salt (inorganic only) |
| hydroxy | succinimide |
| imidazole | sulphide |

| | |
|--------------|-------------------------|
| imide | sulphonate ^a |
| mercaptan | sulphurized |
| methacrylate | thiadiazole |
| naphthenate | thiocarbamate |
| nitrate | triazole |

Notes:

- a. For some product groups, e.g. sulphonate, phenate and salicylate detergents, it is necessary to distinguish between 'overbased' and 'non-overbased' (or 'normal') products. 'Overbased' means that the product contains additional metal carbonate in micellar form, usually described in terms of TBN (total base number), this being the equivalent milligrams of KOH per gram of detergent.
- b. Also known as phenoxyate 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:

Using the concepts of the ATC nomenclature system as set out above, the following are internationally recognized names for current major petroleum additives:

5.1 Zinc and Other Oxyphosphorus Additives:

Zinc alkaryl dithiophosphate

Zinc alkyl dithiophosphate

5.2 Other Metal-based Additives:

Barium long-chain alkaryl sulphonate

Calcium long-chain alkaryl sulphonate

Calcium long-chain alkyl phenate

Calcium long-chain alkyl phenate sulphide

Calcium long-chain alkyl salicylate

Magnesium long-chain alkaryl sulphonate

Magnesium long-chain alkyl phenate sulphide

Magnesium long-chain alkyl salicylate

Sodium long-chain alkaryl sulphonate

5.3 Nitrogen-containing Additives:

Alkyl dithio thiadiazole

Alkyl nitrate

Long-chain alkaryl polyether amidoamine

Long-chain alkylpolyamide amine

Polyalkyl amino phenol

Polyether amide

Polyether amine
Polyolefin amide alkyleneamine
Polyolefin amide alkyleneamine borate
Polyolefin amine

5.4 Sulphides, Phosphorosulphides and Halogen-containing Additives:

Polyolefin phosphorosulphide
Polyolefin sulphide
Long-chain alkyl acid/ester sulphides

5.5 Polymeric Additives:

Alkaryl polyether
Alkyl ester copolymer
Aryl polyolefin
Hydrocarbyl polymer
Long-chain alkaryl polyether
Olefin/alkylester copolymer
Polyalkylene glycol
Poly long-chain alkyl methacrylate
Polyether
Polyolefin
Polyolefin ester

5.6 Other Additives:

Alkylphenol
Long-chain alkane
Long-chain alkaryl sulphonic acid
Long-chain alkyl carboxylic acid
Long-chain alkyl salicylic acid
Long-chain ester
Severely refined virgin mineral oil

6. AUTHORIZED EXTERNAL DISTRIBUTION:

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7. REFERENCES:

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