Making the transition from the IUPAC system

For the most up to date information about INCI nomenclature, visit the CTFA’s Web site at www.ctfa.org.

Every student of organic chemistry is familiar with the IUPAC system of chemical nomenclature. However, one glance at the ingredient listing of a personal-care product can make you wonder why the chemical names are unfamiliar.

Sources for Ingredient Nomenclature

The CTFA (The Cosmetic, Toiletry, and Fragrance Association) did not arbitrarily create ingredient names for the INCI nomenclature system. It relied upon information supplied by chemical vendors and other existing sources of chemical identification.

To prepare a cosmetic product’s ingredient listing, go to the following sources to find the appropriate nomenclature:

1. U.S. Coe of Federal Regulations (21 CFR 701.30) for list of ingredients named by the FDA
2. International Cosmetic Ingredient Dictionary (CTFA) for INCI and Colour Index Names
3. U.S. Pharmacopeia (USP)
4. National Formulary (NF)
5. Food Chemicals Codex (FCC)
6. USAN and the USP Dictionary of Drug Names

Finally, if suitable nomenclature is not found in any of these sources, a technical name or description, or a name that is generally recognizable by consumers may be employed.

Nomenclature Systems

**Semisystematic method:** An older naming system, generally used for low-molecular-weight compounds. Many conventions of this system are used in the INCI system.

**IUPAC (International) System:** Developed by the International Union of Pure and Applied Chemistry, it allows a greater flexibility in naming complex molecules than the semisystematic method
**INCI conventions:** Use simple chemical names whenever possible. Materials that are mixtures of different compounds are named by listing each component ingredient in descending order.

Stem names come from traditional stem names and combinations of traditional stem names when consistent with other systems. USAN abbreviations are use for families of complex ingredients (as PVP for polyvinylpyrrolidone). For compounds that are multiply substituted, use different prefixes; appropriate prefixes include “di-,” “tri-,” or “tetra-.”

**Background**

In the early 1970s, the U.S. cosmetics industry became concerned about government regulation. To demonstrate its capability for self-regulation, it instituted programs to encourage voluntary registration of cosmetic formulations and to scientifically review the safety and efficacy of cosmetic ingredients.

The Cosmetic, Toiletry, and Fragrance Association (CTFA), the major trade and lobbying association for the industry, also realized that standardized ingredient labeling was key to self-regulation. Therefore, it compiled a comprehensive list of all known cosmetic ingredients and assigned ingredient names to be adopted throughout the industry.

**Table 1: IUPAC Hydrocarbon Stem Names**

<table>
<thead>
<tr>
<th>Carbons (main chain)</th>
<th>IUPAC stem term</th>
<th>INCI fatty acids</th>
<th>INCI fatty alcohols</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>Hexane</td>
<td>Capric</td>
<td>Hexyl</td>
</tr>
<tr>
<td>7</td>
<td>Heptane</td>
<td>Heptanoic</td>
<td>Heptyl</td>
</tr>
<tr>
<td>8</td>
<td>Octane</td>
<td>Caprylic</td>
<td>Carylyl</td>
</tr>
<tr>
<td>9</td>
<td>Nonane</td>
<td>Pelagronic</td>
<td>Nonyl</td>
</tr>
<tr>
<td>10</td>
<td>Decane</td>
<td>Capric</td>
<td>Decyl</td>
</tr>
<tr>
<td>11</td>
<td>Undecane</td>
<td>Undecanoic</td>
<td>Undecyl</td>
</tr>
<tr>
<td>12</td>
<td>Dodecane</td>
<td>Lauric</td>
<td>Lauryl</td>
</tr>
<tr>
<td>13</td>
<td>Tridecane</td>
<td>Tridecanoic</td>
<td>Tridecyl</td>
</tr>
<tr>
<td>14</td>
<td>Tetradecane</td>
<td>Myristic</td>
<td>Myristyl</td>
</tr>
<tr>
<td>15</td>
<td>Pentadecane</td>
<td>Pentadecanoic</td>
<td>Pentadecyl</td>
</tr>
<tr>
<td>16</td>
<td>Hexadecane</td>
<td>Palmitic</td>
<td>Cetyl</td>
</tr>
<tr>
<td>17</td>
<td>Heptadecane</td>
<td>Margaric</td>
<td>Heptadecyl</td>
</tr>
<tr>
<td>18</td>
<td>Octadecane</td>
<td>Stearic</td>
<td>Stearyl</td>
</tr>
<tr>
<td>19</td>
<td>Nonadecane</td>
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<td>20</td>
<td>Eicosane</td>
<td>Arachidic</td>
<td>Arachidyl</td>
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<tr>
<td>21</td>
<td>Heneicosane</td>
<td></td>
<td></td>
</tr>
<tr>
<td>22</td>
<td>Docosane</td>
<td>Behenic</td>
<td>Behenyl</td>
</tr>
</tbody>
</table>
This effort produced the CTFA’s *Cosmetic Ingredient Dictionary*. First published in 1973, the dictionary was adopted by the U.S. Food and Drug Administration (FDA) as the official U.S. cosmetic ingredient nomenclature. In view of the nomenclature’s 1994 adoption for international use, the system was renamed the International Cosmetic Ingredient (INCI) system.

The INCI System

To learn the INCI system, it is best to familiarize yourself with the stem terms used to describe the alkyl portions of common cosmetic ingredients, such as fatty acids and alcohols. In general, INCI terms are taken from common chemical terms and therefore may differ from IUPAC’s names for the same alkyl group (see Table 1).

**Stems:** In the INCI system, a fatty acid is named by identifying the longest carbon chain. For example, a 12-carbon straight-chain fatty acid, dodecanoic acid under IUPAC labeling, is lauric acid under the INCI system.

To name a fatty alcohol, name the molecule’s alkyl portion but replace the IUPAC “-ol” with “alcohol.” Thus, a 16-carbon, straight-chain alcohol is not hexadecanol but cetyl alcohol. The INCI naming of branched-chain fatty acids and alcohols follows a convention of adding the prefix “iso-“ to the stem name. For example, the IUPAC name for one 18-C, branched-chain carboxylic acid is 16-methylheptadecanoic acid. However, all 18-C branched carboxylic acids are isostearic acid in the INCI system, regardless of their branching.

**Special Stems:** Cosmetic ingredients often use raw materials that are a complex mixture of alkyl groups rather than a single fatty-chain material. When coconut oil is reacted to make fatty alcohol, the resultant product is, in fact, a combination of various fatty alcohols. Instead of naming each alkyl group present, a stem term is used to reflect the source material. In this case, the fatty alcohols derived from coconut oil would be called coconut alcohol. Similarly “soybean,” “tallow” and “palm kernel” describe alcohols derived from these natural oils.

**Derivatives:** Derivatives, such as ethers and esters, can be named once the alkyl stem has been designated. Remember that an ester is composed of two hydrocarbon chains linked to an oxygen by single bonds. To name an ether, name each alkyl group and add “ether.” Thus an 18-C (stearyl) chain linked to a 16-C (cetyl) chain by an oxygen is stearyl cetyl ether.

Esters are the product of a carboxylic acid reacting with a fatty alcohol. They are named in three parts: the alkyl stem of the alcohol, the stem indicating the acid.
and the suffix “-ate.” Thus, the ester formed by the reaction of cetyl alcohol and palmitic acid is cetyl palmitate.

**Alkanolamides:** Alkanolamides are commonly used in this industry. They are named by combining the alkyl amide stem with an abbreviation for groups attached to the amide portion. Lauramide, for instance, is a merger of a 12-C alkyl group and an amide. If the nitrogen is substituted with an additional alkyl group such as –CH₂CH₂OH, we now have lauramide DEA, where “DEA” (diethanolamine) denotes another attachment.

Quaternized ammonium salts are another class of fatty acid derivative. They are linked to a tri-substituted ammonium ion and thus maintain a positive charge. They are named by adding the suffix “-ium” to the stem of the cation and following with the anion. In most cases, either “-monium,” “dimonium” or “trimonium” is attached to the name, depending on the number of methyl groups (as in cetrimonium chloride). The more complex “quaternium” quaternized salts use an arbitrary number to distinguish between molecules.

Polymerized glycols (epoxides) can be sued independently as cosmetic ingredients or combined with fatty materials to create new derivatives. Under the IUPAC system, or combined with fatty materials to create new derivatives. Under the IUPAC system, polymerizing ethylene oxide forms polyethylene oxide, but polyethylene glycol using INCI Epoxide polymer names use “glycol” to indicate that the molecule has an –OH bond at each end. A number that indicates the degree of polymerization reflects either the molecular weight of the molecule or the moles of epoxide in the polymer. The INCI system abbreviates polyethylene glycol as “PEG” and polypropylene glycol as “PPG.” A polymer with an average 10 moles of ethylene oxide would be PEG-10.

These polymers can be further derivatized. Esters reacted with fatty acids are named like other esters, by identifying the alcohol portion followed by the acid name with the suffix “-ate.” The reaction of a 2-molar PEG polymer with lauric acid yields PEG-2 laurate. Ethers formed by reaction with an alcohol are named by adding the suffix “-eth” to the alcohol stem and indicating the moles of epoxide in the polymeric portion. Thus, the reaction of PEG-20 with cetyl alcohol produces ceteth-20.

An important INCI convention is the use of “ampho-“ with the stem name for the linked alkyl group (thus, sodium cocoaamphoacetate) to describe amphoteric surfactants (zwitterions). Use “imadazoline” when naming alkyl imidazolines that are not amphoteric (e.g. cetyl hydroxyethyl imidazoline).
Silicones: Not all cosmetic ingredients are based on fatty acid chemistry. Silicon-based ingredients, common in personal-care products for lubrication, moisturization and conditioning have their own special nomenclature. As an example, the structure of dimethicone would be hard to deduce from its INCI name alone. Dimethicone (or dimethyl-polysiloxane) is a mixture of fully methylated linear siloxane polymers end-blocked by trimethylsiloxy units. The industry uses literally hundreds of other silicon derivatives based on this chemistry. These include dimethicone copolyol (dimethicone with polyoxyethylene groups added to improve water solubility) and cyclomethicone (cyclic dimethyl polisiloxane) known for its lubricity and volatility.

Ethanol: Alcohols are another cosmetic raw material with specialized nomenclature requirements. Chemists unfamiliar with the INCI system might presume that ethanol would be one of the easiest ingredients to name. Wrong! Because the ethanol employed in most cosmetic products contains some form of denaturant, naming requires specialization.

In fact, the *International Cosmetic Ingredient Dictionary* does not show “ethanol” *per se*. Instead, it displays a list of “specially denatured alcohols” (SDA), each with an abbreviation to specify the denaturant. Ethanol denatured with t-butyl alcohol and sucrose octaacetate is SDA 40-A, but ethanol with methyl alcohol is SDA 3-A. In all, the fifth edition of the dictionary lists 26 denatured alcohols. In the European Union, “alcohol denat” refers to denatured ethanol using an additive approved by the appropriate member states.

Colorants: INCI colorant nomenclature depends upon the regulatory status of the subject material. Most synthetic pigments used in cosmetics are regulated in the U.S. by the FDA. These, known as certified color, have difficult and unwieldy chemical names. Fortunately, INCI classification abbreviates colorants according to their approved usage in either the FD&C (Food, Drug and Cosmetic) D&C (Drug and Cosmetic) or Ext. D&C (External Drug and Cosmetic) certification. Examples include FD&C blue no. 1 (for which common names are brilliant blue or food blue 2), D&C green no. 5 (alizarine cyanine green) and Ext. D&C yellow no. 7 (naphthol yellow S).

In the EU, colorants are identified in the Colour Index (CI) by an internationally recognized 5-digit code. The CI nomenclature is now being listed by CTFA as an alternate INCI name. Thus, FD&C blue no. 1 is also CI 42090.
Some classes of colorant, not requiring special certification, are identified differently. Two common examples are the iron oxides (such as cosmetic black and cosmetic brown) and the ultramarine colors (ultramarine blue, pink and green). Color-imparting cosmetics frequently use these insoluble pigments.

Basic dyes are primarily used as permanent or semipermanent hair colorants. Examples include basic blue 9, also known as 3,7-bis(dimethylamino)phenothiazin-5-ium chloride and basic brown 16, or [8-(p-aminophenyl)azo]-7-hydroxy-2-napthyl]trimethylammonium chloride.

**Other ingredients:** Though there appears to be an endless number of chemical designations and abbreviations, the INCI system also uses many easily recognizable names for natural and natural-derived ingredients. These include beeswax, lanolin, menthol and a host of other animal-, vegetable- and mineral-derived components.

The manner in which INCI names are assigned to so-called natural materials depends upon their composition. Materials of biological origin, such as “hyaluronic acid” are named by specific terms once they have been isolated and purified.

When the exact components in a mixture can not be reasonable classified, as with certain plant extracts, the source may be used to name the material. “Aloe vera,” for example, identifies the material extracted from the plant of the same name. Other noteworthy examples include keratin protein, vegetable gums, and various mineral waxes. Such familiar terms ease the obvious difficulty of assigning IUPAC names to materials that are mixtures of many compounds.

Fragrances are designated by the comparatively mundane and non-descriptive qualifier “fragrance” though they may be elaborate concoctions of exotic elements like Siberian pine needles, whale musk and rose petal extract. No further chemical id is required. However, in circumstances where specific aroma chemicals are cited on ingredient statements, the INCI nomenclature should be used. For example, “chamomile” is the name given to the fragrance oil extracted from the plant of the same name.

If an ingredient is considered to be proprietary or a trade secret, its vendor can petition the FDA to allow that material to be listed as simply “other ingredients” on labeling for the U.S. market. In addition, if an incidental material is present that has no function or effect on the formula, or if it is present at an insignificant level, it need not be declared on the ingredient listing.

Water, perhaps the most common of all cosmetic ingredients, can only be legally identified as “water.”