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Hydrocarbons

Vicente L. Cebolla and Luis Membrado Giner
CSIC, Zaragoza, Spain

I. HYDROCARBON SAMPLES

Hydrocarbons occur together with other related compounds as complex mixtures in nature (e.g., petroleum) and human activities (e.g., products derived from the conversion of petroleum, coal, shale, and oil). Likewise, hydrocarbons are ubiquitous pollutants in soils, water, and air, and some of them have carcinogenic and/or mutagenic activities.

The composition of these mixtures, as well as the occurrence of a particular hydrocarbon family, depends on the type of sample and its source or process history. In the case of environmental samples, it also depends on the method and extent of sample cleanup. As a consequence of this, the composition of hydrocarbon-containing samples varies in molecular structure and size, polarity, and functionality or chemical group.

Hydrocarbon types found in real samples can be summarized as saturates (*n*-alkanes, isoalkanes, and cycloalkanes), olefins (alkenes and cycloalkenes), monoaromatics, polycyclic aromatic hydrocarbons (PAHs, hydrocarbons containing two or more rings of the benzenoid structure), and condensed hydroaromatic structures (1). Furthermore, heterocyclic (N, S, O) aromatic structures —compounds with PAH structure in which carbon atoms have been substituted with oxygen, sulfur, or nitrogen atoms—occur together with PAHs in many cases. The presence of these compounds is so common in hydrocarbon-containing samples that it is customary to refer to all aromatic compounds as polycyclic aromatic compounds (PACs) instead of PAHs. In addition to the cited compounds, other types of polar molecules can be found together with hydrocarbons depending on the origin of the sample. These include nitroaromatics; condensed aromatics with phenolic, ketonic, or carboxylic groups; and others in environmental samples or even as porphyrins in heavy petroleum residues or fullerenes from fossil fuel combustion samples.

This picture becomes more complicated as the sample boiling range becomes higher due to the increase in the number of isomers for each family, the increase in concentration of polar compounds, and the increasing number of possible combinations of compound types (e.g., alkylaromatics).

Apart from the samples derived from fossil sources, hydrocarbons can also be found in samples derived from organic reactions or synthesis (e.g., fullerenes) or other natural products (e.g., terpene hydrocarbons).

II. TYPES OF ANALYSES REQUIRED

Given that complete molecular separation of the components of hydrocarbon-containing samples is not usually possible owing to their complex nature and the limitations of current separation techniques, the types of analysis required for these samples include either the determination of targeted, individual hydrocarbons or the separation and quantification of hydrocarbon types (2). The latter is commonly required in industry at either the analytical or semipreparative scale. In