STRUCTURAL CLASSIFICATION AND CHARACTERIZATION OF HEAVY PETROLEUM BASE OIL HYDROCARBONS BY GC×GC-HR-TOF/MS

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Base oil, the major component of lubricant (about 80%), is an essentially complex mixture of highly abundant saturated hydrocarbons that are generally refined from heavy petroleum fractions. The increasing demand for higher capacity lubricants is driven by expanding industrial plants that require optimum friction reductions. There is now clear potential for the comprehensive structural elucidation of hydrocarbon classes and functionalized biomarkers in heavy base oil for effective use and formulation of performance enhanced lubricants. Understanding the complex molecular composition by mapping their distribution in various base oil fractions can help tune refinery processes to develop appropriate product quality target as well as to develop new additive packages.

Recent applications of comprehensive two-dimensional gas chromatography to light petroleum fractions were demonstrated to be a powerful tool yielding enhanced resolution for several classes. However, limited information is available on the applicability of comprehensive GC for heavy base oil fractions. Moreover, those FID based detection techniques were found to be inconclusive and insufficient to resolve full spectrum of hydrocarbons due to the sample's enormous complexity as well as due to lack of mass spectrometric information.

The objective of this study is set to assess the applicability of GC×GC coupled with HR-TOF/MS for characterization of several groups of base oils. Setting the chromatographic conditions to the limits to elute high boiling base oils considered earlier as unamenable to GC×GC, complimented by the proprietary chromatographic accessories, methods has been developed to provide solutions for comprehensive profiling for heavy base oils. Starting from sample introduction, columns, modulators to cutting edge ionization and detection techniques were evaluated. Experimental design based method optimization, automation in high resolution data treatment and synthesis (CLIC, mass defect) and further multivariate statistical assay were performed to provide in depth view of base oil and will be discussed.