

COMPREHENSIVE TWO-DIMENSIONAL GAS CHROMATOGRAPHY COMBINED WITH HIGH-RESOLUTION MASS SPECTROMETRY: EXPLORING MASS DEFECT INFORMATION TO CHARACTERIZE BASE OIL

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High-resolution mass spectrometry (HR-MS) offers much more than separation of chemically distinct constituents in a complex mixture such as base oil used for lubricant formulations. Since each nuclide has a different mass defect, each ion of different elemental composition has a different mass. Moreover, each additional ring or double bond decreases the number of hydrogens by 2, it is possible to determine the compound “type” from the number of hydrogens relative to carbons. Thus, it becomes possible to recognize a series of compounds of the same class and type, but different extent of alkylation, by finding a series of mass spectral peaks differing by 14.01565 Da in mass. The Kendrick scale effectively converts the mass of CH₂ from 14.01565 to exactly 14.00000. Thus, homologous series will have identical Kendrick mass defect (KMD).

GC×GC coupled with HR-TOF MS offer the best possible separation of their respective techniques. However, such experiments yield enormous data sets that require new informatics tools to facilitate the interpretation of the rich information content. Current work deals with the analysis of several groups of base oil comprising several hydrocarbon classes including highly abundant saturated hydrocarbons namely paraffinic, naphthenic compounds as well as olefins and aromatic compounds. In essence, application of KMD analysis for complex hydrocarbon mixtures greatly simplifies the HR-MS data handling because homologous compounds share the same KMD. The mass defect plot served as a visual aid from which different alkylation series are recognizable on the basis of their mass defect. KMD derived data was further used in the analysis and chemical fingerprinting of base oil samples. This was further aided by multivariate analysis based on KMD revealing discrimination efficiencies for several groups of base oils.