Virtual Gas Chromatography of Gasoline

comparison with ASTM chromatograms

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Temperature Programmed Gas Chromatograms are calculated and compared to measured reference chromatograms. Separation science of Giddings and Golay is used for peak time and peak width prediction. Input is the TPGC method and an excel file with isothermal Kovats indices[1] on DB-1 and DB-5, molecular formula, and name label of 230 compounds:

Detailed Hydrocarbon Analysis of spark-ignition fuel has peak purity issues that prompted ASTM to adopt 4 Temperature Programmed Gas Chromatography methods for DHA, namely D 6729, D 6730, D 6733#1 and D 6733#2. Reference separations and coelutions are predicted by VGC from Kovats & density input in Excel KovatsPhenylMethylSilicone.csv

StillPeaks Virtual GC software can predict separations and coelutions from input of TPGC conditions and a Kovats index spreadsheet. Start using the dimensionless isothermal Kovats index, which is independent of length, diameter and film thickness[1] and download Virtual GC from: www.StillPeaks.com

Isothermal Kovats index on Dimethylsilicone, viscosity of **G** phase & **L** phase and *T*, *n*-Alkane CH_4-*n*C_{14} solubility in **L** and vapor pressure (API 44) result in TPGC peaks: