A Solution for Determination of High-Concentration Aromatic Compounds in Finished Gasolines Satisfying ASTM D5769 Using a New Benchtop GC-TOFMS

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Introduction

ASTM D5769 is a widely accepted standard method used in the petroleum industry for determination of benzene, toluene, and total aromatics in finished gasolines by GC-MS. A common difficulty encountered with this method is the concern with saturation of the ion source, which leads to nonlinearity in calibration curves, especially for the quantification of the high-concentration aromatics, such as toluene. LECO’s Pegasus® BT GC-TOFMS easily satisfies the method requirements for sensitivity, ion ratios, and calibration linearity, providing a solution for analysis of the aromatic compounds listed in ASTM D5769 without saturation of the ion source. Calibration curves were built for the standard method analytes and then applied to samples with the addition of semi-quantification for similar analytes on a sample of 93-octane gasoline, as stipulated in the method.

Methods

The Pegasus BT GC-TOFMS easily met all requirements necessary to properly analyze a finished gasoline sample for total aromatics. All 23 calibrated analytes are labeled in the chromatogram in Figure 3. Results for the commercial 93 octane gasoline fell within the expected ranges of 0.09 to 4% for benzene at 0.2%, 1.0 to 13% for toluene at 1.44%, and 9 to 42% for total aromatics determined at 10.75%.

Calibration Linearity

- Benzene: 0.99992
- Toluene: 0.99980
- Ethylbenzene: 0.99998
- 1,2-Dimethylbenzene: 0.99998
- Benzene, 1-ethyl-2-methyl-: 0.99998
- Benzene, propyl-: 1.00000
- Benzene, 1,2,4-trimethyl-: 1.00000
- Benzene, 1,2-diethyl-: 0.99992
- Benzene, 1,2,3-trimethyl-: 1.00000
- Naphthalene: 1.98
- Naphthalene, 2-methyl-: 0.36
- Uncalibration C12-Benzene: 0.01
- Uncalibrated C11-Benzenes: 0.19
- Uncalibrated Indans: 2.82
- Total Aromatics: 10.75

Conclusions

In order to meet the requirements for using ASTM D5769 to characterize a sample, three fundamental mass spectrometer criteria must be met: sensitivity for 1.4-diethylbenzene, achieving specified ion abundance ratios for key masses of 1,2,3-trimethylbenzene, and calibration linearity for all analytes. After all method criteria were successfully completed, a sample of commercially available 93-octane gasoline was analyzed. Automatic Peak Find with deconvolution provided all the necessary information to determine total aromatics.