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SUPELCO®

Application Note 53

Highly Characterized Reference Standard: Heavy Straight Run Naphtha

A straight run naphtha, or gasoline, is produced from crude oil by distillation, typically in the temperature range of 60-320°F. Light straight run naphtha is the distillate fraction collected at 60-170°F; heavy straight run naphtha typically is collected at 170-320°F. Heavy straight run naphtha is a hydrotreating or reforming base (feed) stock. Straight run naphthas usually have low octane numbers.

Key Words

• naphtha • reference standard • distillation

The reference standard described here is not an artificial mixture of components, but is a "real world" sample, taken from a distillation tower prior to the reforming unit. Thus it reflects the composition of typical high boiling naphthas analysts are likely to encounter. Carefully analyzed by GC/FID and GC/MS procedures, this new standard is intended for use as both a qualitative and quantitative reference standard. Analysts can use the chromatograms and peak identifications shown here and enclosed with the product as guide maps for evaluating specific naphthas. We anticipate that this reference standard will be used for evaluating refinery process performance, for identifying sources of contamination, in method development, in PIANO analyses, and in training.

To prepare this standard, we obtain bulk samples of heavy straight run naphtha from a petroleum refinery and package the material under nitrogen in amber ampuls. We evaluate packaging homogeneity in our QA department, using randomly selected ampuls from the beginning and end of every packaging run. If the homogeneity evaluations are satisfactory, we send samples to an outside evaluator, Consolidated Sciences Inc. (Pasadena, Texas, USA) for detailed component analysis (Figure A).

Consolidated Sciences' analytical approach provides both quantitative data, based on flame ionization detection, and qualitative information, using a mass spectrometer as the detect0r (Figure B). Use of an "open split" interface between the column and mass spectrometer mimics FID retention times throughout the analysis and prevents vacuum effects on separations.

Quantitative data are reported on the basis of area percent (Figure A), as a common ground for all to compare, to preclude controversy over whether liquid or weight percent constitutes proper results and what are proper response factors. Area percent can be measured with reasonable accuracy and precision, while liquid and weight percent determinations depend on response factors and on the use of pure analytical standards, many of which are unavailable.

Samples used for this reference standard are analyzed in a unique manner: they are separated into aromatic and saturate fractions, using silica gel column chromatography. Each fraction is analyzed separately, using a polar (Carbowax®) gas chromatography column, then the fractions are recombined mathematically, based on analysis of key aromatic components. Loss of lighter components, which occurs in the silica gel separation, is corrected by using the data generated from the original sample. Thus, we provide three chromatograms with the standard: one for the original sample, one for the aromatic fraction, and one for the saturate fraction.

Figure A. Portion of the Analysis Report for Naphtha Reference Standard

Petroleum Refinery Heavy Straight Run Naphtha
Cat # 47488
Lot # LA40360

Ret. Time	Component	Class	Mol. Wt.	Area %
8.12	n-Butane	P	58	0.004
9.35	Isopentane	P	72	0.029
10.02	n-Pentane	P	72	0.066
11.28	2,2-Dimethylbutane	P	86	0.004
12.57	Cyclopentane	N	70	0.021
12.65	2,3-Dimethylbutane	P	86	0.016
12.86	2-Methylpentane	P	86	0.128
13.66	3-Methylpentane	P	86	0.100
14.74	n-Hexane	P	86	0.342
16.52	2,2-Dimethylpentane	P	100	0.010
16.70	Methylcyclopentane	N	84	0.281
17.00	2,4-Dimethylpentane	P	100	0.023

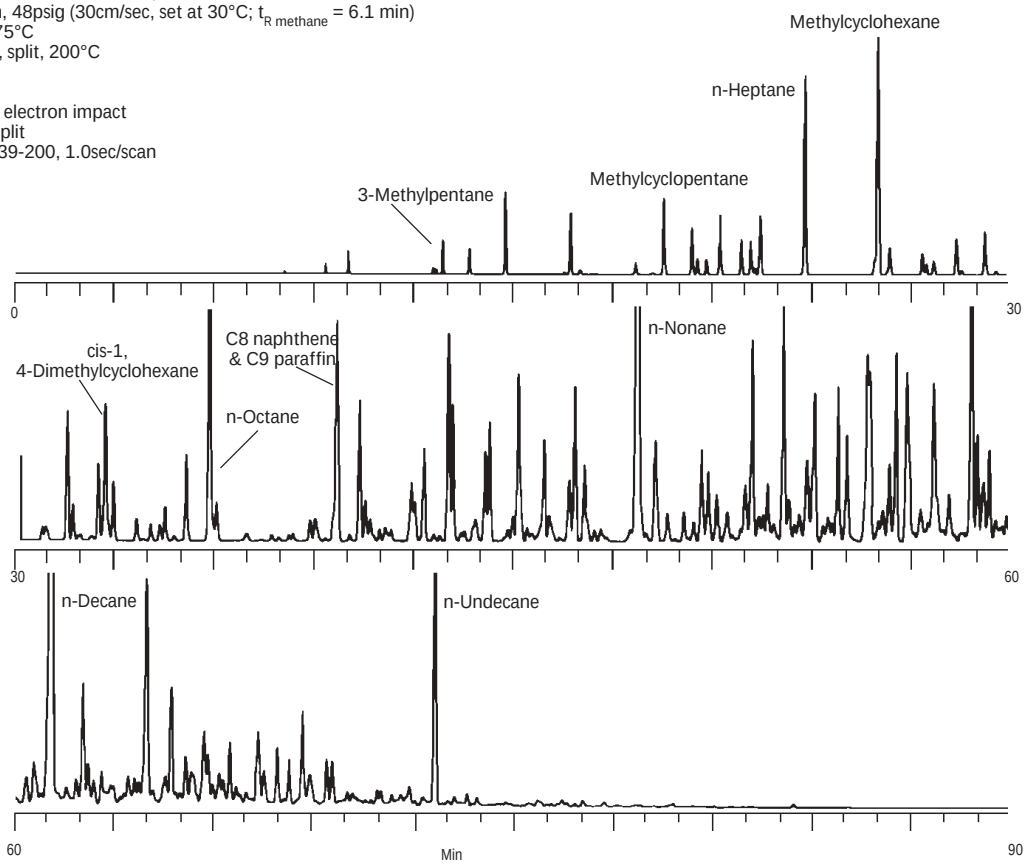
Figure B. Petroleum Refinery Heavy Straight Run Naphtha

Capillary GC/FID

Instrument:	Hewlett-Packard 5890, Series II
Column:	**Petrocol DH, 100m x 0.25mm ID, 0.5µm film**
Cat. No.:	**24160-U**
Col. Temp.:	35°C (10 min) to 150°C at 1.5°C/min, then to 280°C at 5°C/min, hold 15 min
Carrier:	helium, 48psig (30cm/sec, set at 30°C; $t_{R\ methane}$ = 6.1 min)
Det.:	FID, 275°C
Inj.:	0.1mL, split, 200°C

MS Parameters

Ionization Energy:	70 eV, electron impact
Interface:	open split
Scan:	m/z = 39-200, 1.0sec/scan



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The temperature programming and linear velocity (pressure) parameters chosen are known to be suitable for a wide range of petroleum stream samples encountered by Consolidated Sciences. The analysis is isobaric, although pressure programming could be used. The head pressure used allows good separation of early eluting components and reasonable linear velocity over a wide temperature range.

In the information included with this standard, molecular weights are provided in all cases where they are measurable (Figure A). Along with fragmentation patterns, these values are helpful for identifying less common components. Isomers are identified when possible; total carbon number is given when further identification is not possible. Some paraffin/naphthene coelutions are known to occur. Mass spectra and corresponding signal strengths for ions in these two hydrocarbon classes are used to estimate the degree of coelution. The error in this estimate is less than 10%.

If your work involves analyses of naphthas, we feel this reference standard will be an important tool for you.

Ordering Information:

Description	Cat. No.
Heavy Straight Run Naphtha Reference Standard 1mL	**47488**
Petrocol™ DH Capillary Column 100m x 0.25mm ID fused silica, 0.50µm film	**24160-U**

Trademarks
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