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Application Note 52

Highly Characterized Reference Standard: Reformate

Catalytic conversion at temperatures of 850-1000°F converts – reforms – low-octane naphthas into high-octane products for gasoline and aviation fuel blending and aromatic concentrates. The predominant reaction during reforming is the dehydrogenation of naphthenes (cycloparaffins) to the corresponding aromatics. For example, cyclohexane reforms to benzene, and methylcyclohexane reforms to toluene. Research Octane Numbers can be increased from the low 40s to over 100 through reforming.

Key Words

● reformate ● reference standards ● naphthenes ● aromatics

Carefully analyzed by GC/FID and GC/MS procedures, this 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 reformates. 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 reformate 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 detector (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. A preliminary class separation of the saturate and combined aromatic/olefin fractions assures proper mass spectral identification of olefins and naphthenes.

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.

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).

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

Petroleum Refinery Reformate
Cat # 47489
Lot # LA40361

Ret. Time	Component	Class	Mol. Wt.	Area %
7.62	Isobutane	P	58	0.010
7.95	n-Butane	P	58	0.110
8.11	2,2-Dimethylpropane	P	72	0.002
8.25	cis-2-Butene	O	56	0.001
8.78	3-Methyl-1-butene	O	70	0.004
9.16	Isopentane	P	72	1.570
9.50	1-Pentene	O	70	0.003
9.68	2-Methyl-1-butene	O	70	0.010
9.81	n-Pentane	P	72	0.960
10.03	trans-2-Pentene	O	70	0.009
10.28	cis-2-Pentene	O	70	0.006
10.45	2-Methyl-2-butene	O	70	0.030
11.04	2,2-Dimethylbutane	P	86	0.450
11.79	Cyclopentene	O	70	0.008
11.94	4-Methyl-1-pentene	O	84	0.004

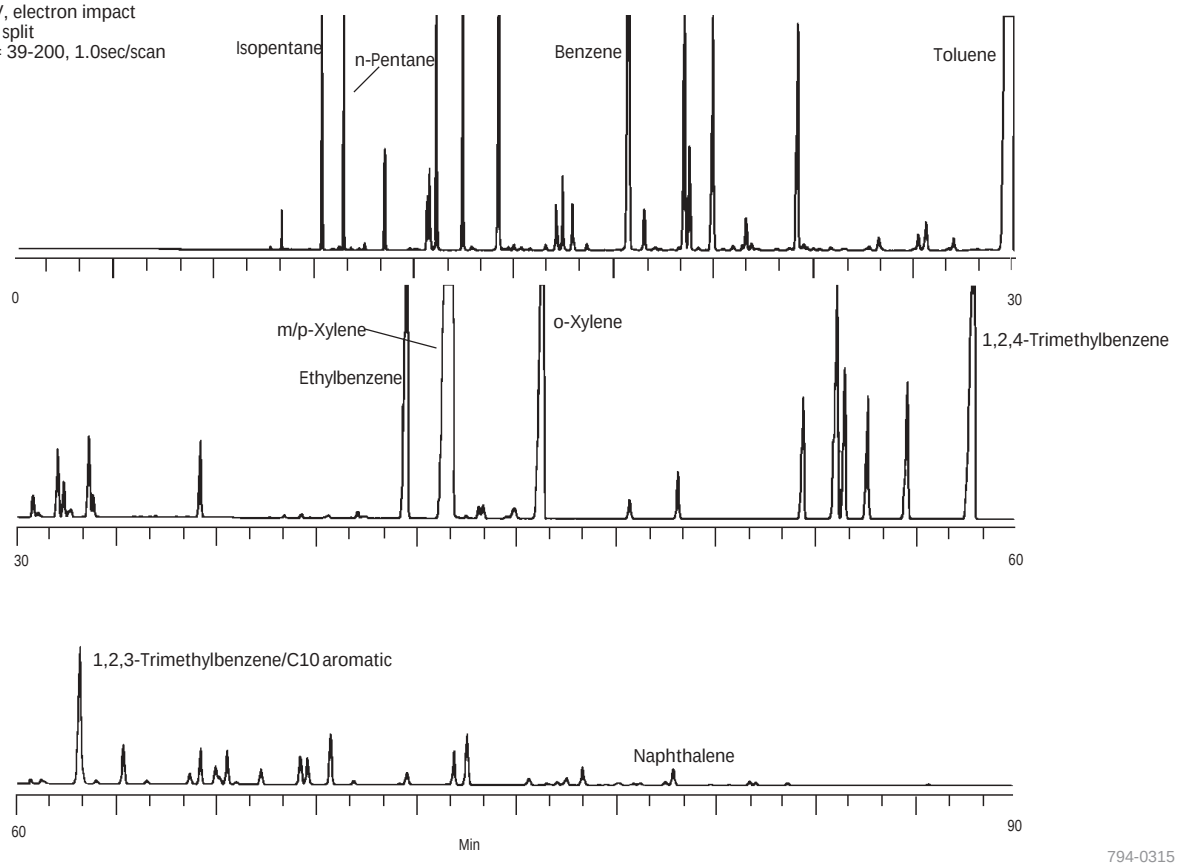
Figure B. Petroleum Refinery Reformate

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



794-0315

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. However, confidence in the hydrocarbon class assay exceeds 95%. Cases of coelution are dealt with by estimation, based on mass spectral signal strength.

If your work includes monitoring hydrocarbon streams or other analyses involving reformates, we highly recommend this reference standard to you.

Ordering Information:

Description	Cat. No.
Petroleum Refinery Reformate Reference Standard	
1mL	**47489**
Petrocol™ DH Capillary Column	
100m x 0.25mm ID fused silica, 0.50µm film	**24160-U**

Fused silica columns manufactured under HP US Pat. No. 4,293,415.

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