PETROCHEMICAL

New Rtx-1 PONA Column for Analysis of Petroleum Products

Gasoline is a complex mixture containing hundreds of individual hydrocarbons including alkanes (paraffins), alkenes (oletins), cyclic alkanes (naphthenes) and aromatics. Using high resolution gas chromatography (HRGC), it is possible to resolve and identify over two hundred individual components in a single analysis. Once the hydrocarbons are identified and quantified, the results can be reported in various ways including: detailed hydrocarbon analysis (DHA), hydrocarbon type analysis, and special calculations such as vapor pressure and octane number. Because the task of calibrating hundreds of peaks is extremely time consuming, committees such as the American Society of Standards and Materials (ASTM) and the Canadian General Standards Board (CGSB) have developed standardized methodology for detailed hydrocarbon analysis(1,2)*. These methods specify a 100 meter column which must be reproducible if laboratories are to obtain accurate results. The Restek Rtx-1PONA column meets or exceeds the demanding resolution and retention time requirements specified in these methods.

An example of HRGC analysis of unleaded gasoline using the Rtx-1PONA column appears in Figure 1. The detailed report obtained from this analysis contain over 200 individual peaks so identification of each component can be very challenging. Since flame ionization detection is specified, identification of the individual components is practical only if the retention times and separations are comparable to those published in the ASTM or CGSB methods. In order to meet these demanding resolution and retention criteria, Restek has developed unique quality control tests and specifications for the Rtx-1PONA column. The measured values for retention (k), efficiency (n) and stationary phase selectivity (RI) are controlled so that each column exceeds the requirements of the ASTM and CGSB methods. These requirements include separating several "critical pairs" of closely eluting peaks of different hydrocarbon classes. Figure 2 illustrates three of these critical separations obtained from the analysis of gasoline, without the need for cryogenic cooling.

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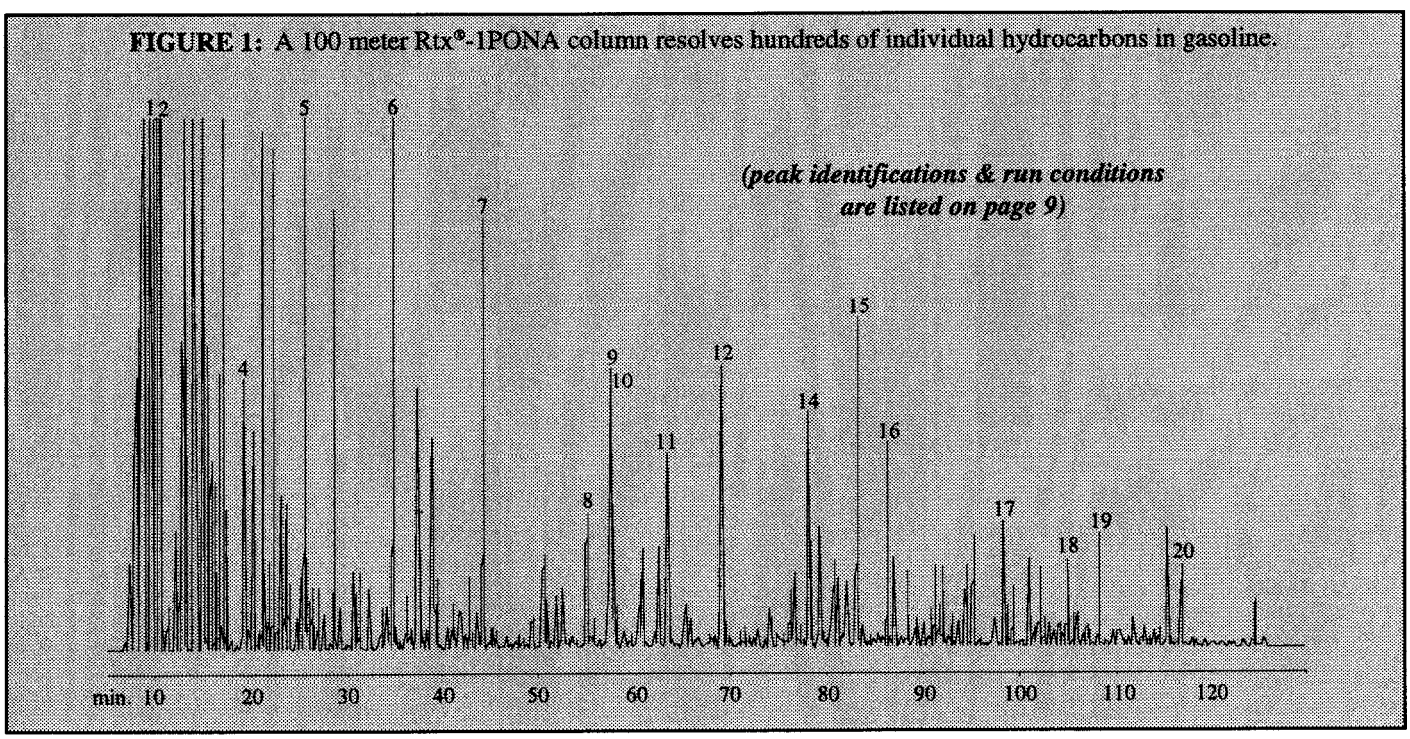
Detailed hydrocarbon analysis provides a great deal of information regarding the chemical composition of gasoline and similar petroleum products. This information is useful in evaluating the performance of a refinery process or to calculate the chemical "value" of a particular hydrocarbon stream

FIGURE 1: A 100 meter Rtx®-1PONA column resolves hundreds of individual hydrocarbons in gasoline.



(peak identifications & run conditions are listed on page 9)

[1]N.G. Johanson, Proposed ASTM Test Method for Detailed Hydrocarbon Analysis, Draft 2, ASTM Committee D2.04.
*Canadian General Standards Board, ***Methods of Testing Petroleum*** and ***Associated Products 3.0,*** Method No. 14.3-94 (Feb 94).

for chemical production or gasoline blending. It is possible to summarize the detailed chromatographic report into a hydrocarbon type analysis utilizing a computer program and a table listing the carbon number and type of each calibrated peak. Table I is an example of a PIONA report obtained from an unleaded gasoline using a BASIC program written for a programmable integrator. It is also possible to develop correlations for other important properties such as vapor pressure and octane number from the compositional analysis of gasoline and naphtha3. A 100 meter column is also specified for petrochemical analyses[4] requiring a high degree of resolution, where specialized stationary phases or column switching systems do not achieve the desired separations.

The Rtx- 1PONA column is an excellent choice for separation of complex petroleum products such as gasoline and naphtha. Each column is specially tested to exact specifications, to meet the demanding separation and retention criteria of the ASTM and CGSB procedures. With HRGC it is possible to resolve and identify hundreds of individual hydrocarbons and this information can be useful for hydrocarbon type (PIONA) analysis or for estimating vapor pressure and octane number.

Run Conditions for Figures 1 & 2

100m, 0.25mm ID, 0.50µm
Rtx®-1PONA (cat.# 10156)
SAMPLE: 0.5µl split injection of unleaded gasoline
OVEN TEMP.: 35°C (hold 13 min.) to 45°C @ 10°C/min. (hold 15 min.), to 60°C @ 1.0°C/min. (hold 15 min.), to 200°C @ 1.9°C/min. (hold 5 min.)
INJ. TEMP.: 250°C, **DET. TYPE:** FID,
DET. TEMP.: 250°C
CARRIER GAS: helium
LINEAR VELOCITY: 24 cm/sec. set @ 35°C
FID SENSITIVITY: 4 x 10^{-12} AFS
SPLIT RATIO: 100:1

Compound List for Figure 1

1 **ethanol**	**11** o-xylene
2. pentane	12. nonane
3. hexane	13. propylbenzene
4. benzene	14. I-methyl-3-ethylbenzene
5. heptane	15. 1,2,4&methylbenzene
6. toluene	16. decane
I. octane	17. undecane
8. ethylbenzene	18. naphthalene
9. m-xylene	19. dodecane
10 p-xylene	20. tridecane

FIGURE 2: Resolution of several critical pairs of hydrocarbons.

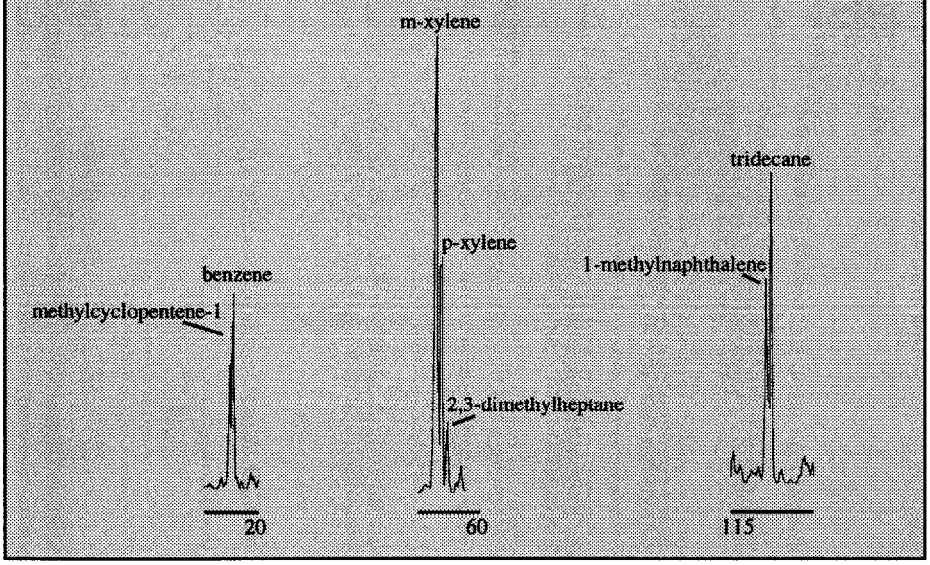


TABLE I: Hydrocarbon Type Report from Detailed Hydrocarbon Analysis

C#	P(Wt%)	I(Wt%)	O(Wt%)	N(Wt%)	A(Wt%)	X(Wt%)
2	.00	.00	.00	.00	.00	3.48
3	.07	.00	.00	.00	.00	.23
4	.24	.20	.83	.00	.00	.21
5	1.80	8.77	8.76	.12	.00	.00
6	1.84	4.93	4.21	1.88	.64	.00
7	2.14	4.31	2.93	3.95	2.66	.0
8	2.42	4.24	.70	3.85	5.31	.06
9	1.72	3.86	.36	3.19	5.27	.15
10	.88	2.61	.04	.62	4.72	.36
11	.48	.47	.00	0.17	1.63	.12
12	.43	.61	.00	.02	.56	.29
13	.30	.34	.00	.00	.00	.00
Total	12.34	30.34	17.83	13.82	20.78	4.90

Coming Soon.. .

"Oxygenates in Gasoline"

according to ASTM Method D4815. The article will include application chromatograms and product listings for columns and new chemical standards.

3R.P. Walsh and J.V. Mortimer, ***Hydrocarbon Processing,*** p. 153 September 197 1.
4ASTM D5441 Standard Test Method for the Analysis of Methyl Tert-Butyl Ether (MTBE) by Gas Chromatography, ***Annual Book of Standards,*** Vol. 5.03