# Trace Impurities in Monocyclic Aromatic Hydrocarbons

- PAC Aromatics impurity analyzer meets & exceeds ASTM requirements
- Delivered as factory tested, calibrated, and validated analyzer
- Based on the robust and reliable Agilent 8890 GC platform


**Keywords**: Aromatics, ASTM D7504, impurities

## Introduction:

Almost all aromatics, so called because of their distinctive perfumed smell, come from crude oil, although small quantities are made from coals. The main substances in this group are benzene, toluene, and xylenes. They are used as starting materials for a wide range of consumer products: clothing, pharmaceuticals, cosmetics, computers, paints, vehicle components, cooking utensils, household fabrics, sports equipment, etc. Products made using aromatics can reduce energy consumption and so have a positive impact on the environment. (Source: www.aromaticsonline.eu).

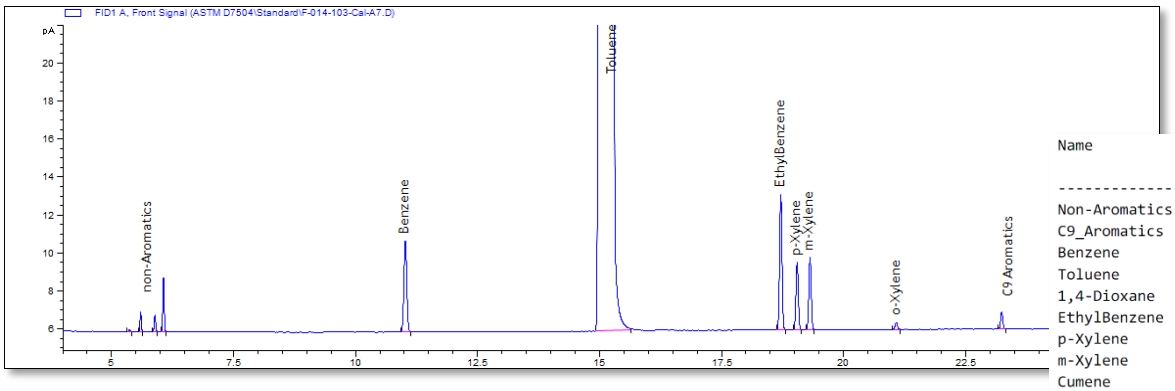
Determining the type and amount of hydrocarbon impurities remaining from the manufacture of toluene, mixed xylenes, p-xylene, o-xylene, ethylbenzene, benzene, and styrene used as chemical intermediates and solvents is often required. One of the test methods describing this impurity testing is ASTM D7504 (which can be seen as the new alternative for the superseded ASTM D5917)

The "Significance and Use" of D7504 states that the test method is suitable for setting specifications and for use as an internal quality control tool where these products are produced or are used. Typical impurities are alkanes containing 1 to 10 carbons atoms, benzene, toluene, ethylbenzene (EB), xylenes, and aromatic hydrocarbons containing nine carbon atoms or more.

## Analysis

PAC Powered by AC offers a guaranteed and turn-key analyzer, as part of its analyzer portfolio for petrochemical industry, that meets all the requirements as listed in ASTM D7504.

The analyzer is configured with a split inlet (S/SI), polar capillary column (PEG) and Flame Ionization Detector (FID). For the sample introduction the system is equipped with an Automatic Liquid Sampler (ALS). After injection the capillary column separates the individual components in a temperature-programmed oven run. See example chromatogram & report below:




| Name | Total Area [pA*s] | Norm % |
|---|---|---|
| Non-Aromatics | 9.61414 | 8.724e-3 |
| C9_Aromatics | 2.90251 | 2.457e-3 |
| Benzene | 19.53104 | 0.0161 |
| Toluene | 1.19774e5 | 99.9297 |
| 1,4-Dioxane | 0.00000 | 0.0000 |
| EthylBenzene | 24.69154 | 0.0208 |
| p-Xylene | 12.14635 | 0.0102 |
| m-Xylene | 13.06225 | 0.0110 |
| Cumene | 0.00000 | 0.0000 |
| o-Xylene | 1.25187 | 1.053e-3 |
| Totals : | | 100.0000 |

## Quantification:

For the quantification of the identified components the peak area is measured and adjusted using "Effective Carbon Number" (ECN) factors as listed in table 2 of the method. The concentration of each component is using the following formula:

$$C_i = 100 * (A_i * R_i) / \sum_{i=1}^{n} (A_i * R_i)$$

where:

$C_i$ = concentration for component i, mass %,

$A_i$ = peak area of component i

$R_i$ = ECN correction factor for component i

Volume concentration can be calculated using the density of each individual component (listed in the same table).

This method may not detect all components and there may be unknown components that would be assigned in appropriate correction factors and thus, the results may not be absolute.

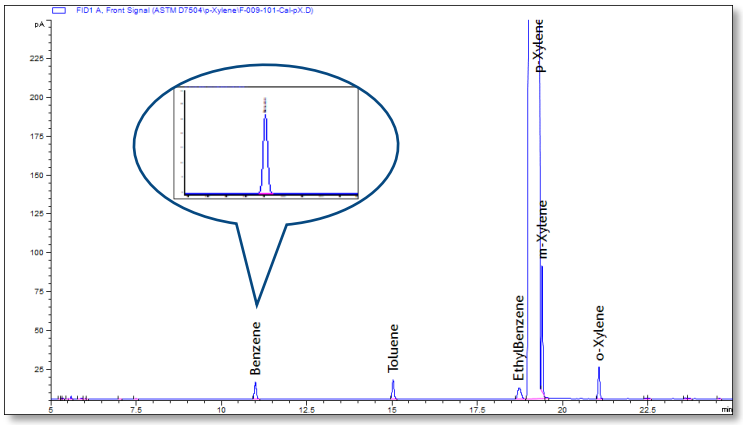
## Limit of detection:

The limit of detection is specified by the method at 0.0002% mass (equals 2 mg/kg) and the quantification limit at 0.0006% mass (equals 6 mg/kg) for impurities in benzene, toluene, (mixed-) xylenes, ethylbenzene, and styrene.

LDL's are calculated according to the formula: LDL = (( 3 * c * N ) / A ) * W * 60

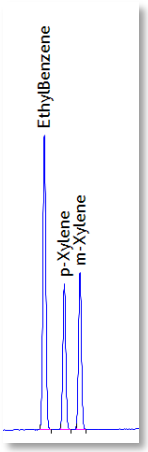
| | | |
|---|---|---|
| LDL | = | Lower detection limit ( ppm weight ) |
| c | = | Concentration of component of interest ( ppm weight ) |
| N | = | Noise ( peak to peak ) ( pA ) |
| A | = | Area of peak of interest ( pA * s ) |
| W | = | Width of peak at half height (minutes) |

The analyzer meets and exceeds this performance requirements for every detected components, see below chromatogram:



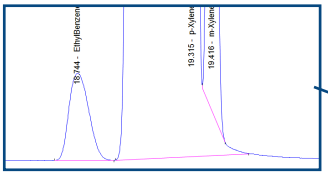

*Impurities in p-Xylene at an approximate concentration of 10 mg/kg.*

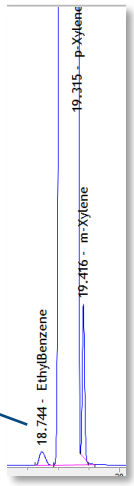
## Separation & Interferences




One of the other requirements of the method is an adequate separation of Ethylbenzene & para-Xylene should either one of them be the product that is to be analyzed. The criteria is that "the distance from the baseline to the valley between the two peaks is not greater than 50% of the peak height of the lower of the two peaks". The graph to the left clearly shows that the system meets the requirement with ease.

The graph to the right shows the required adequate separation of m-xylene & p-xylene.






## Conclusion

With the "Trace Impurities in Monocyclic Aromatic Hydrocarbons" analyzer according to ASTM D7504 PAC offers an analyzer for the petrochemical industry that meets and exceeds all requirements as listed by the method. With the factory test and application guarantee on PAC's analyzers, the customer does not have to spend time developing methods and can rest assured that the analyzer can be used from day one with the certainty that the application is set up correctly.

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