

APPLICATIONS

TN-2094 Optimal Separation of PAH Compounds including Chrysene & Triphenylene using Zebron™ ZB-PAH-CT GC column

Ramkumar Dhandapani and Rola Elabaji
Phenomenex, Inc., 411 Madrid Ave., Torrance, CA 90501 USA



Ramkumar Dhandapani, Ph.D.
Product Manager - Gas Chromatography

He has a PhD in Analytical Chemistry and over 15 years experience in chromatographic method development and troubleshooting. Ramkumar loves to write poems, read Shakespeare, and attend Shakespeare plays.

Introduction

Polycyclic aromatic hydrocarbons (PAHs) are carcinogenic substances that must be monitored in food and environment as per local regulations. There are numerous PAH compounds that have structural similarities including Chrysene and Triphenylene that are hard to resolve on a traditional GC column. Chromatographically, there are 3 components that contribute to improve resolution of peaks. It comprises of Efficiency term, Selectivity term, and Retention term. Among the three terms, Selectivity is most influential in drastic resolution improvement. For optimal resolution of Chrysene and Triphenylene, several combinations of stationary phases were explored. Presented in this study is an optimal stationary phase Zebron ZB-PAH-CT that was utilized for separation of EU 15+1 PAHs along with Triphenylene to evaluate overall separation of PAH and separation of critical pairs Chrysene and Triphenylene.

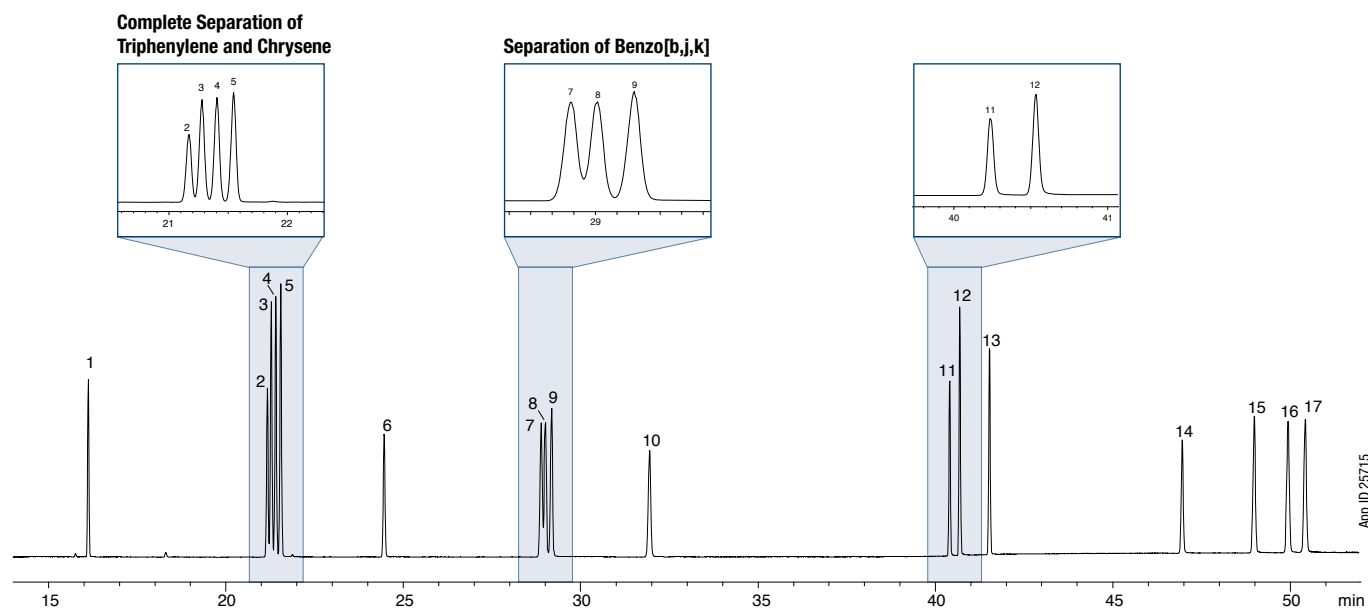
Figure 1.
Master Resolution Equation

$$R_s = \frac{\sqrt{N}}{4} \times \frac{\alpha - 1}{\alpha} \times \frac{k}{k + 1}$$

Efficiency
Selectivity
Retention

$N = \text{theoretical plates}$
 $\alpha = k_2/k_1$
 $k = (t_R - t_0)/t_0$

Figure 2.
EU 15+1 PAH and Triphenylene on a Zebron ZB-PAH-CT GC column

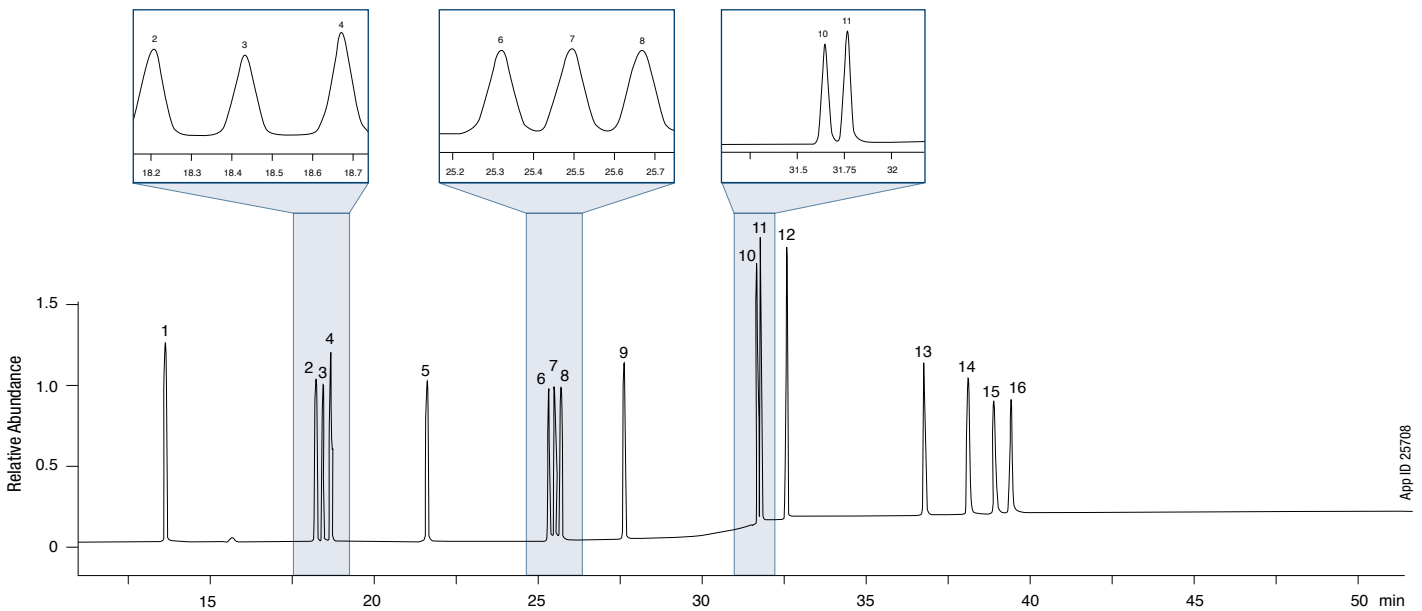


Column: Zebron ZB-PAH-CT
Dimensions: 40 meter x 0.18 mm x 0.14 μm
Part No.: 7PD-G044-47
Injection: Split 30:1 @ 320 °C, 1 μL
Recommended Liner: Zebron PLUS Single Taper Z-Liner™
Liner Part No.: AG2-4B13-05 (for Shimadzu® 2010 GC)
Carrier Gas: Helium @ 78 psi (constant pressure)
Oven Program: 45 °C for 0.8 min to 200 °C @ 45 °C/min to 265 °C @ 3 °C/min for 5 min to 270 °C @ 1 °C/min to 320 °C @ 10 °C/min for 15 min
Detector: MSD (Shimadzu® GC-MS-QP2010 Ultra)
Mode: SIM
SIM Ions: 216, 226, 228, 242, 252, 276, 278, 302 m/z
Transfer line Temperature: 300 °C
Source Temperature: 300 °C

Sample:

- | | |
|--------------------------|-----------------------------|
| 1. Benzo[c]fluorene | 10. Benzo[a]pyrene |
| 2. Cyclopenta[c,d]pyrene | 11. Indeno[1,2,3-c,d]pyrene |
| 3. Benz[a]anthracene | 12. Dibenzo[a,h]anthracene |
| 4. Triphenylene | 13. Benzo[g,h,i]perylene |
| 5. Chrysene | 14. Dibenzo[a,i]pyrene |
| 6. 5-Methylchrysene | 15. Dibenzo[a,e]pyrene |
| 7. Benzo[b]fluoranthene | 16. Dibenzo[a,i]pyrene |
| 8. Benzo[j]fluoranthene | 17. Dibenzo[a,h]pyrene |
| 9. Benzo[k]fluoranthene | |

Figure 3.
EU 15+1 PAH on a Zebron ZB-PAH-EU GC column



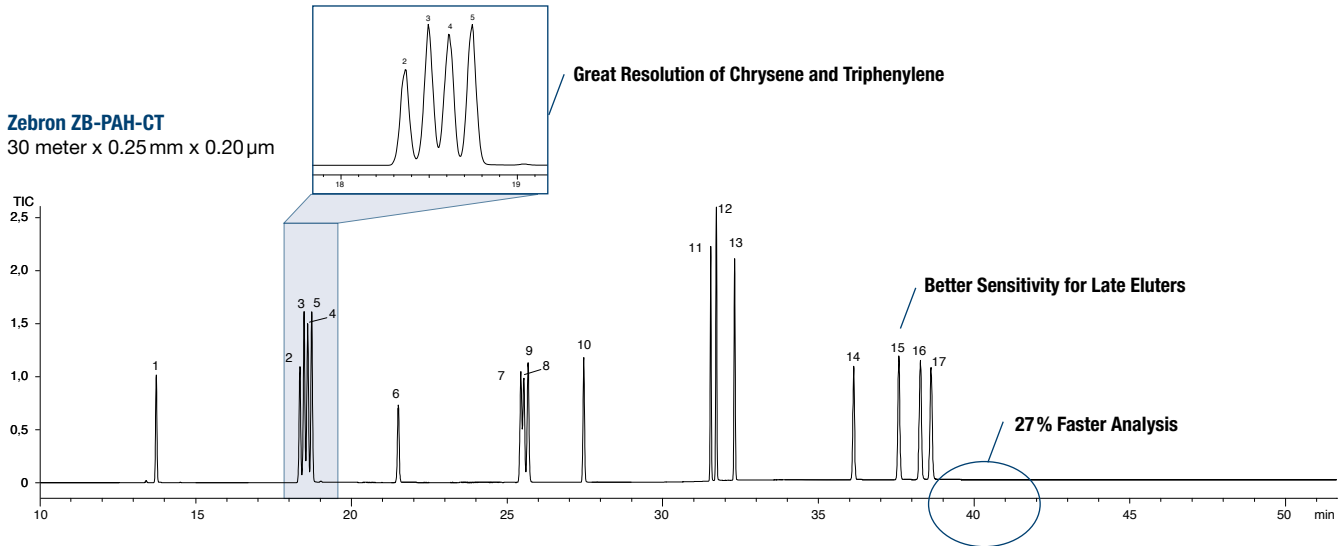
App ID 25708

Column: Zebron ZB-PAH-EU
Dimensions: 30 meter x 0.25 mm x 0.20 μ m
Part No.: [ZHG-G043-10](#)
Injection: Split 5:1 @ 330 °C, 1 μ L
Recommended Liner: Zebron PLUS Single Taper Z-LinerSM
Liner Part No.: [AG2-4B13-05](#) (for Shimadzu[®] 2010 GC)
Carrier Gas: Helium @ 24 psi (constant pressure)
Oven Program: 45 °C for 0.8 min to 200 °C @ 45 °C/min to
 226 °C @ 3 °C/min for 0 min to 320 °C @
 10 °C/min for 20 min
Detector: MSD, 50-500 m/z
Transfer line Temperature: 300 °C
Source Temperature: 300 °C

Sample:

1. Benzo[c]fluorene
2. Benz[a]anthracene
3. Cyclopenta[c,d]pyrene
4. Chrysene
5. 5-MethylChrysene
6. Benzo[b]fluoranthene
7. Benzo[k]fluoranthene
8. Benzo[j]fluoranthene
9. Benzo[a]pyrene
10. Indeno[1,2,3-cd]pyrene
11. Dibenzo[a,h]anthracene
12. Benzo[g,h,i]perylene
13. Dibenzo[a,i]pyrene
14. Dibenzo[a,e]pyrene
15. Dibenzo[a,l]pyrene
16. Dibenzo[a,h]pyrene

Figure 4.
Comparison of Analysis of EU 15+1 PAHs and Triphenylene



GC-MS conditions for both applications:

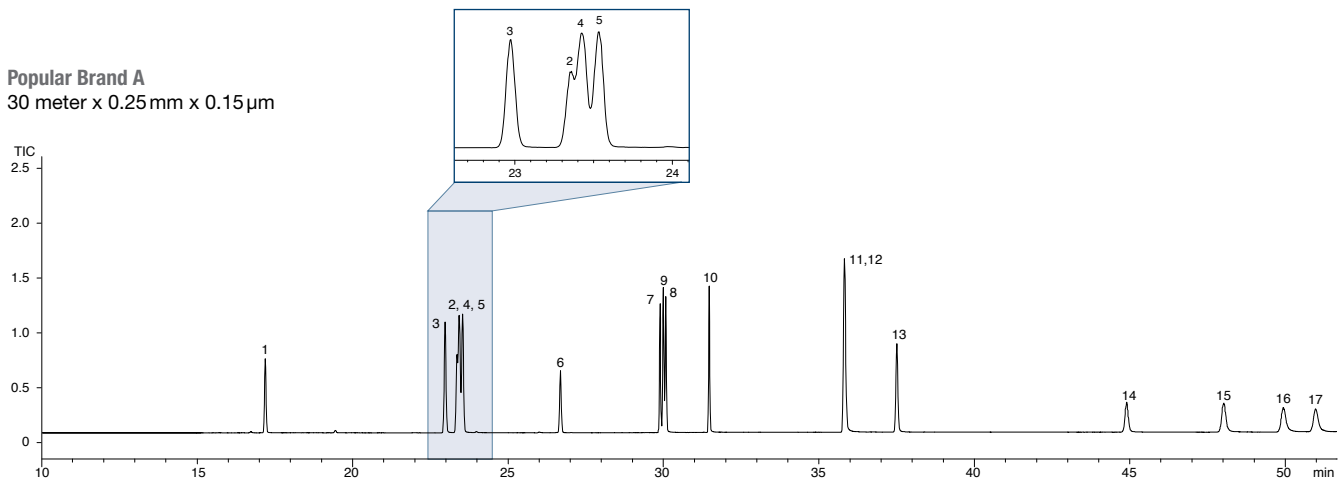
Column: As Indicated
Dimensions: As Indicated
Part No.: [7HG-G044-10](#) (Zebtron ZB-PAH-CT)
Injection: Split 15:1 @ 320 °C, 1 μL
Recommended Liner: Zebtron PLUS Single Taper Z-Liner™
Liner Part No.: [AG2-4B13-05](#)
Carrier Gas: Helium @ 23.7 psi (constant pressure)
Oven Program: 45 °C for 0.8 min to 200 °C @ 45 °C/min to 266 °C @ 3 °C/ min for 0 min to 320 °C @ 10 °C/ min to 320 °C for 20 min
Detector: MSD (Shimadzu® GC-MS-QP2010 Ultra)
Mode: SIM
SIM Ions: 216, 226, 228, 242, 252, 276, 278, 302 m/z
Transfer line Temperature: 300 °C
Source Temperature: 300 °C

Sample:

1. Benzo[c]fluorene
2. Cyclopenta[c,d]pyrene
3. Benz[a]anthracene
4. Triphenylene
5. Chrysene
6. 5-Methylchrysene
7. Benzo[b]fluoranthene
8. Benzo[j]fluoranthene
9. Benzo[k]fluoranthene
10. Benzo[a]pyrene
11. Indeno[1,2,3-c,d]pyrene
12. Dibenzo[a,h]anthracene
13. Benzo[g,h,i]perylene
14. Dibenzo[a,i]pyrene
15. Dibenzo[a,e]pyrene
16. Dibenzo[a,l]pyrene
17. Dibenzo[a,h]pyrene

VS.

Popular Brand A
30 meter x 0.25 mm x 0.15 μm



Comparative separations may not be representative of all applications.

APPLICATIONS

Results and Discussion

Separation of PAH isomers are quite challenging as there are many PAH components that have structural similarities. Specifically, Chrysene and Triphenylene are one such hard to separate critical pairs. In the present study, unique selectivity of ZB-PAH-CT was utilized to resolve EU 15+1 and Triphenylene. As shown in **Figure 2**, the 40 meter x 0.18 mm x 0.14 μm ZB-PAH was able to completely resolve Chrysene from Triphenylene. In addition, ZB-PAH-CT also provided a peak order switch for certain PAH analytes compared to ZB-PAH-EU, including Benz[a]anthracene, Cyclopenta[c,d]pyrene (Peak 2 and 3 in **Figure 2** and 3); Benzo[b,j,k]fluoranthene (Peak 7, 8, 9 in **Figure 2** and peak 6, 7, 8 in **Figure 3**) due to the unique selectivity. The selectivity change and enhanced resolution of Chrysene and Triphenylene helps avoid false positives in the analysis. In addition to resolving Chrysene and Triphenylene completely, ZB-PAH-CT in a 40 meter dimension provided the highest resolution of 2.6 for Benzo[b,k]fluoranthene

Further, EU 15+1 and Triphenylene mix was evaluated on a 30 meter ZB-PAH-CT and 30 meter Popular Brand A GC column under identical chromatographic conditions. As shown in **Figure 4**, ZB-PAH-CT shows better resolution of Chrysene and Triphenylene, better sensitivity for heavy PAH, and 27% faster run time because of the unique stationary phase selectivity.

Conclusion

Zebtron ZB-PAH-CT provides complete resolution of Chrysene and Triphenylene in addition to other EU 15+1 PAHs with a 40 meter column dimension. In addition to providing great resolution of Chrysene and Triphenylene, ZB-PAH-CT provides high resolution for Benzo[b,k]fluoranthene, gives better sensitivity for heavy PAH, and provides 27% faster run time than common PAH GC columns.

Ordering Information

Zebtron™ ZB-PAH-CT GC Column

| Length (meter) | ID (mm) | df (μm) | Temp. Limits (°C) | Part No. |
|----------------|---------|----------------------|-------------------|-----------------------------|
| 20 | 0.18 | 0.14 | 40 to 320/340 | 7FD-G044-47 |
| 30 | 0.25 | 0.20 | 40 to 320/340 | 7HG-G044-10 |
| 40 | 0.18 | 0.14 | 40 to 320/340 | 7PD-G044-47 |

Zebtron™ ZB-PAH-EU GC Column

| Length (meter) | ID (mm) | df (μm) | Temp. Limits (°C) | Part No. |
|----------------|---------|----------------------|-------------------|-----------------------------|
| 10 | 0.10 | 0.08 | 40 to 340/360 | 7CB-G043-59 |
| 20 | 0.18 | 0.14 | 40 to 340/360 | 7FD-G043-47 |
| 30 | 0.25 | 0.20 | 40 to 340/360 | 7HG-G043-10 |
| 60 | 0.25 | 0.20 | 40 to 340/360 | 7KG-G043-10 |

BE-HAPPY™
guarantee

Your happiness is our mission. Take 45 days to try our products. If you are not happy, we'll make it right.
www.phenomenex.com/behappy

Australia

t: +61 (0)2-9428-6444
auinfo@phenomenex.com

Austria

t: +43 (0)1-319-1301
anfrage@phenomenex.com

Belgium

t: +32 (0)2 503 4015 (French)
t: +32 (0)2 511 8666 (Dutch)
beinfo@phenomenex.com

Canada

t: +1 (800) 543-3681
info@phenomenex.com

China

t: +86 400-606-8099
cninfo@phenomenex.com

Denmark

t: +45 4824 8048
nordicinfo@phenomenex.com

Finland

t: +358 (0)9 4789 0063
nordicinfo@phenomenex.com

France

t: +33 (0)1 30 09 21 10
franceinfo@phenomenex.com

Germany

t: +49 (0)6021-58830-0
anfrage@phenomenex.com

India

t: +91 (0)40-3012 2400
indiainfo@phenomenex.com

Ireland

t: +353 (0)1 247 5405
eireinfo@phenomenex.com

Italy

t: +39 051 6327511
italiainfo@phenomenex.com

Luxembourg

t: +31 (0)30-2418700
nlinfo@phenomenex.com

Mexico

t: 01-800-844-5226
tecnicomx@phenomenex.com

The Netherlands

t: +31 (0)30-2418700
nlinfo@phenomenex.com

New Zealand

t: +64 (0)9-4780951
nzinfo@phenomenex.com

Norway

t: +47 810 02 005
nordicinfo@phenomenex.com

Poland

t: +48 22 104 21 72
pl-info@phenomenex.com

Portugal

t: +351 221 450 488
ptinfo@phenomenex.com

Singapore

t: +65 800-852-3944
sginfo@phenomenex.com

Spain

t: +34 91-413-8613
espinfo@phenomenex.com

Sweden

t: +46 (0)8 611 6950
nordicinfo@phenomenex.com

Switzerland

t: +41 (0)61 692 20 20
swissinfo@phenomenex.com

Taiwan

t: +886 (0) 0801-49-1246
twinfo@phenomenex.com

United Kingdom

t: +44 (0)1625-501367
ukinfo@phenomenex.com

USA

t: +1 (310) 212-0555
info@phenomenex.com

☎ All other countries/regions

Corporate Office USA
t: +1 (310) 212-0555
info@phenomenex.com



www.phenomenex.com

Phenomenex products are available worldwide. For the distributor in your country/region, contact Phenomenex USA, International Department at international@phenomenex.com

Terms and Conditions

Subject to Phenomenex Standard Terms and Conditions which may be viewed at www.phenomenex.com/TermsAndConditions.

Trademarks

Zebtron, Z-Liner, and Be-Happy are trademarks of Phenomenex. Shimadzu is a registered trademark of Shimadzu Corporation.

FOR RESEARCH USE ONLY. Not for use in clinical diagnostic procedures.

© 2020 Phenomenex, Inc. All rights reserved.