

Application Note # CA-270380

Paraffins, Iso-Paraffins, Naphthenes and Aromatics (PINA) in Hydrocarbon Streams

Introduction

This application note describes the quantitative determination of paraffins, iso-paraffins, naphthenes and aromatics (PINA) in spark ignition fuels by the multi-dimensional gas chromatography separation approach utilized in the Bruker PIONA+™ Analyzer.

The Bruker PIONA+ Analyzer is a comprehensive GC system that offers the ability to characterize and quantify the components in a variety of spark ignition fuels according to an array of industry standard method protocols. The system is highly flexible and can be operated in one of multiple method modes depending on the analysis requirements for a given stream type. For this application, the system was set up to characterize the PINA content of spark ignition fuels.

Instrumentation:

Bruker PIONA+ Analyzer

CompassCDS Chromatography Software from Bruker with PIONA+ plug-in software

Table 1: Elution scheme for PINA.

| From | To (min) | Components | Column route |
|------|----------|-------------------|---|
| 0 | 30.0 | C1 to C12 N + P | 1 st OV-275 fraction 13x |
| 30.0 | 35.0 | C6 to C8 A and pN | 2 nd OV-275 fraction via arom/eth to non-polar column |
| 35.0 | 40.0 | >200 °C fraction | Back flush non-polar column of 2 nd OV-275 fraction |
| 50.0 | 80.0 | C3 to C12 nP | 5A in flow to 13x |
| 80.0 | 86.5 | C8 to C10 A | 3 rd back flush OV-275 fraction via arom/eth to non-polar column |
| 86.5 | 95.0 | >200 °C fraction | Back flush non-polar column of 3 rd OV-275 fraction |

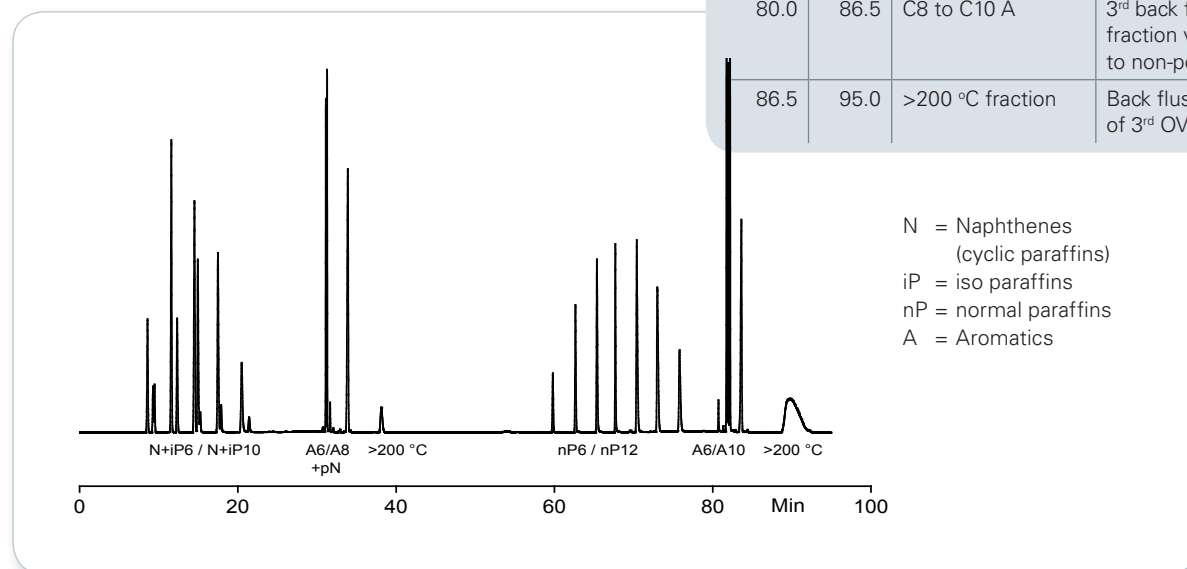


Figure 1: Chromatogram of test sample 1.

Conditions

All conditions for the different columns and traps are set in order to obtain the elution pattern outlined in Table 1.

Results and discussion

The chromatogram in Figure 1 shows the analysis of test sample 1. This sample is used to calibrate the analyzer. The component grouping is very clear, making identification and quantification easy and accurate. From the chromatogram the PIONA+ software generates reports. Weight% and volume% profile reports are shown in Tables 2 and 3. The paraffins, iso-paraffins, naphthenes and aromatics are grouped and reported per carbon number and as totals. Furthermore, totals per carbon number are reported.

Another example of a PINA analysis is shown in Figure 2. This chromatogram shows a reformer feed, a fairly simple sample containing hydrocarbons from C6 to C11. From this chromatogram, CompassCDS software with the PIONA+ plug-in generate weight% and volume% profile reports as shown in table 4 and 5. Thus, in one overview, the amounts of the different groups, naphthenes, iso-paraffins, paraffins and aromatics, are reported. In addition, the totals per group and per carbon number are displayed.

Conclusion

The Bruker PIONA+ Analyzer successfully analyzed paraffins, iso-paraffins, naphthenes and aromatics in a calibration sample and a reformer feed. The PIONA+ Analyzer provided comprehensive mass% and volume% reports.

Table 2: Weight% report of the test sample.

Normalized Weight Percent Profile

| Carbon | Naphthenes | Iso-Paraffins | n-Paraffins | Aromatics | Total |
|------------------|------------|---------------|-------------|-----------|-------|
| 2 | | | | | |
| 3 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 4 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 5 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 6 | 2.39 | 1.73 | 1.28 | 2.85 | 8.26 |
| 7 | 5.66 | 2.55 | 2.59 | 2.90 | 13.70 |
| 8 | 5.69 | 4.61 | 3.92 | 10.46 | 24.68 |
| 9 | 4.57 | 0.69 | 3.00 | 6.76 | 15.01 |
| 10 | 2.40 | 0.50 | 5.10 | 5.19 | 13.20 |
| 11 | 0.00 | 0.01 | 4.24 | 0.00 | 4.25 |
| Total | 20.71 | 10.10 | 20.24 | 28.17 | 79.22 |
| Fraction >200 °C | | 14.31 | | | |
| Polynaphthenes | | 6.65 | | | |

Table 3: Volume% report of the test sample.

Normalized Volume Percent Profile

| Carbon | Naphthenes | Iso-Paraffins | n-Paraffins | Aromatics | Total |
|------------------|------------|---------------|-------------|-----------|-------|
| 2 | | | | | |
| 3 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 4 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 5 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 6 | 2.45 | 2.03 | 1.51 | 2.51 | 8.49 |
| 7 | 5.80 | 2.88 | 2.92 | 2.58 | 14.15 |
| 8 | 5.77 | 5.05 | 4.30 | 9.32 | 24.33 |
| 9 | 4.55 | 0.73 | 3.20 | 5.98 | 14.39 |
| 10 | 2.25 | 0.53 | 5.40 | 4.52 | 12.74 |
| 11 | 0.00 | 0.02 | 3.92 | 0.00 | 3.93 |
| Total | 20.82 | 11.24 | 21.40 | 24.91 | 78.19 |
| Fraction >200 °C | | 14.83 | | | |
| Polynaphthenes | | 6.98 | | | |

Table 4: Weight% report of the reformer feed.

Normalized Weight Percent Profile

| Carbon | Naphthenes | Iso-Paraffins | n-Paraffins | Aromatics | Total |
|------------------|------------|---------------|-------------|-----------|-------|
| 3 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 4 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 5 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 6 | 0.28 | 0.00 | 0.02 | 0.02 | 0.32 |
| 7 | 8.33 | 2.30 | 4.57 | 1.71 | 16.90 |
| 8 | 19.51 | 12.32 | 11.62 | 5.88 | 49.32 |
| 9 | 12.29 | 11.50 | 5.70 | 1.32 | 30.80 |
| 10 | 0.83 | 0.92 | 0.13 | 0.05 | 1.93 |
| 11 | 0.00 | 0.09 | 0.09 | 0.00 | 0.19 |
| Total | 41.23 | 27.13 | 22.12 | 8.97 | 99.45 |
| Fraction >200 °C | | 0.5 | | | |
| Polynaphthenes | | 0.05 | | | |

Table 5: Volume% report of the reformer feed.

Normalized Volume Percent Profile

| Carbon | Naphthenes | Iso-Paraffins | n-Paraffins | Aromatics | Total |
|------------------|------------|---------------|-------------|-----------|-------|
| 2 | | | | | |
| 3 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 4 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 5 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 6 | 2.44 | 2.03 | 1.51 | 2.51 | 8.49 |
| 7 | 5.77 | 2.88 | 2.92 | 2.58 | 14.15 |
| 8 | 5.66 | 5.05 | 4.30 | 9.32 | 24.33 |
| 9 | 4.48 | 0.73 | 3.20 | 5.98 | 14.39 |
| 10 | 2.30 | 0.53 | 5.40 | 4.52 | 12.74 |
| 11 | 0.00 | 0.02 | 3.92 | 0.00 | 3.93 |
| Total | 20.64 | 11.24 | 21.40 | 24.91 | 78.19 |
| Fraction >200 °C | | 14.83 | | | |
| Polynaphthenes | | 6.98 | | | |

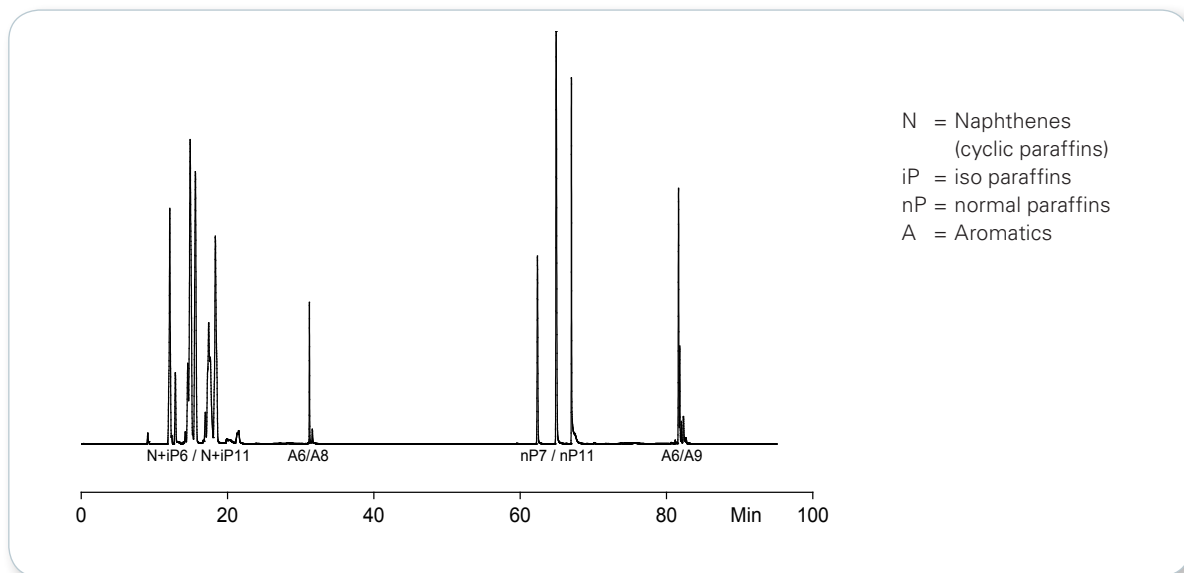


Figure 2: Chromatogram of a reformer feed.

| Keywords |
|----------------------|
| spark ignition fuels |
| Quantitation |
| paraffins |
| iso-paraffins |
| naphthenes |
| aromatics |

| Instrumentation & Software |
|----------------------------|
| Bruker PIONA+ Analyzer |
| PIONA+ plug-in software |
| CompassCDS Software |

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