APPLICATION NOTE AN134

UOP690, C_8 and low boiling paraffins and naphthenes in low-olefin hydrocarbons by GC.

INTRODUCTION

The UOP690 describes the determination method for C_8 and lower boiling paraffins and naphthenes in olefin free gasolines (2 mass-%) with a maximum boiling point of 260°C. In this method benzene and toluene are also being determined.

This method contains two procedures using the same column to determine the resolved non-aromatic components. Depending on the degree of resolution required either method A alone, or both method A and B can be used. Method A looks at a broad spectrum of components while method B zooms in on the lighter components and this data can be used to calculate unresolved non-aromatic components from method A.

Figure 1 shows the SCION Instruments 4X6 GC platforms that can be used for UOP690.

Figure 1. SCION Instruments 4X6 GC

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EXPERIMENTAL

This analysis can be implemented on the 436-GC and the 456-GC platform. The analysis was performed on the Scion 456-GC analyser equipped with an FID and a 100 positions 8400 autosampler.

The UOP 690 is a perfect and simple method for the determination of the mass-% composition of the sample.

A big advantage of running both methods is the possibility for detailed identification by comparing chromatograms of method A and B. With these methods it is possible to determine the unresolved non-aromatic components from method A.

In table 3 the components that have to be determined by analysis A and B can be found.

RESULTS

All the results were calculated according to the described method in UOP690.

The theoretical relative response factors (TRRF) were determined and showed a deviation from the theoretical value below 3% for the components.

In addition it showed that the three measurements performed for these components had a deviation below 1% amongst the results. These results were excellent since the deviation against the theoretical values have to be below 5% and the deviation amongst the results no more than 2%.

After establishing the TRRF a gasoline mix was injected to determine the mass-% . This gasoline mix was analysed with method A and method B.

Both methods showed excellent repeatability that are well withing specifications prescribed in the UOP 690.

Table 1. Analytical conditions of method A

Injector	Splitless 200:1, 250 °C
Column	Scion-DHA-50
Oven Program	32°C (6.0 min), 5°C/min to 52°C (14.0 min) , 20 °C/min to 250°C (9 min)
Carrier	Hydrogen, 1.1 ml/min (*GC equipped with a H_2 sensor bundle)
Detector	FID with ceramic jet, 250°C Air: 300 ml/min, Fuel gas (H_2): 30 ml/min, Make up (N_2): 30 ml/min
Inj. Volume	0.5 µl
Autosampler	8400
Software	Compass CDS

Table 2. Analytical conditions of method B

Injector	Splitless 200:1, 250 °C
Column	Scion-DHA-50
Oven Program	60°C (8.0 min), 5°C/min to 90°C (0 min) , 20 °C/min to 250°C (10 min)
Carrier	Hydrogen, 1.1 ml/min
Detector	FID with ceramic jet, 250°C Air: 300 ml/min, Fuel gas (H_2): 30 ml/min, Make up (N_2): 30 ml/min
Inj. Volume	0.5 µl
Autosampler	8400
Software	Compass CDS

After analysis and calculation of the mass it showed that the sum of all components (resolved and unresolved) was 99.63 mass-%, this means that the data had to be renormalized to 100 mass-%.

An example of the chromatograms from method A and B can be found in figure 2.

* Hydrogen Sensor bundle/safety pack available from Scion Instruments

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Table 3: Components determined with analysis A and B, peak number with letters refer to co-eluting peaks.

Peak Nr. A	Peak Nr. B	Component	Peak Nr. A	Peak Nr. B	Component
1	-	Propane	36	-	3.3-Dimethylhexane
2	-	Isobutane	37	-	1-trans-2-cis-3-Trimethylcyclopentane
3	-	n-Butane	38	-	2.3.4-Trimethylpentane
4	-	2.2-Dimethylpropane	39A	-	2.3.3-Trimethylpentane
5	-	Isopentane	39B	-	Toluene
6	-	n-Pentane	40A	6	2.3-Dimethylhexane
7	-	2.2-Dimethylbutane	40B	7	1.1.2-Trimethylcyclopentane
8	-	Cyclopentane	41	-	2-Methyl-3-ethylpentane
9	-	2.3-Dimethylbutane	42	-	2-Methylheptane
10	-	2-Methylpentane	43	-	4-Methylheptane
11	-	3-Methylpentane	44A	-	3.4-Dimethylhexane
12	-	n-Hexane	44B	-	3-Methyl-3-ethylpentane
13	-	2.2-Dimethylpentane	45A	-	1-cis-2-trans-4-Trimethylcyclopentane
14	-	Methylcyclopentane	45B	8B	1-cis-2-cis-4-Trimethylcyclopentane
15	-	2.4-Dimethylpentane	46	-	3-Methylheptane
16	-	2.2.3-Trimethylbutane	47A	8A	3-Ethylhexane
17	-	Benzene	47B	9A	1-cis-3-Dimethylcyclohexane
18	-	3.3-Dimethylpentane	47C	9B	1-cis-2-trans-3-Trimethylcyclopentane
19	-	Cyclohexane	48	-	1-trans-4-Dimethylcyclohexane
20	-	2-Methylhexane	49	-	1.1-Dimethylcyclohexane
21	-	2.3-Dimethylpentane	50	-	1-Methyl-trans-3-ethylcyclopentane
22	-	1.1-Dimethylcyclopentane	51	-	1-Methyl-cis-2-ethylcyclopentane
23	-	3-Methylhexane	52	-	1-Methyl-trans-2-ethylcyclopentane
24	-	1-cis-3-Dimethylcyclopentane	53	-	1-Methyl-1-ethylcyclopentane
25	-	1-trans-3-Dimethylcyclopentane	54	-	1-trans-2-Dimethylcyclohexane
26	-	3-Ethylpentane	55	-	1-cis-2-cis-3-Trimethylcyclopentane
27	-	1-trans-2-Dimethylcyclopentane	56A	10	n-Octane
28	-	2.2.4-Trimethylpentane	56B	11	1-cis-4-Dimethylcyclohexane
29	-	n-Heptane	56C	12	1-trans-3-Dimethylcyclohexane
30A	2	Methylcyclohexane	57	-	Isopropylcyclopentane
30B	1A	1-cis-2-Dimethylcyclopentane	58	-	1-Methyl-cis-2-ethylcyclopentane
31A	3	1.1.3-Trimethhylcyclopentane	59	-	1-cis-2-Dimethylcyclohexane
31B	1B	2.2-Dimethylhexane	60A	13	n-Propylcyclohexane
32	4A	Ethylcyclopentane	60B	14	Ethylcyclohexane
33		2.5-Dimethylhexane	61	-	Ethylbenzene
34A	5	2.2.3-Trimethylpentane	62A	-	m-Xylene
34B	4B	2.4-Dimethylhexane	62B	-	p-Xylene
35	-	1-trans-2-cis-4-Trimethylcyclopentane	63	-	o-Xylene

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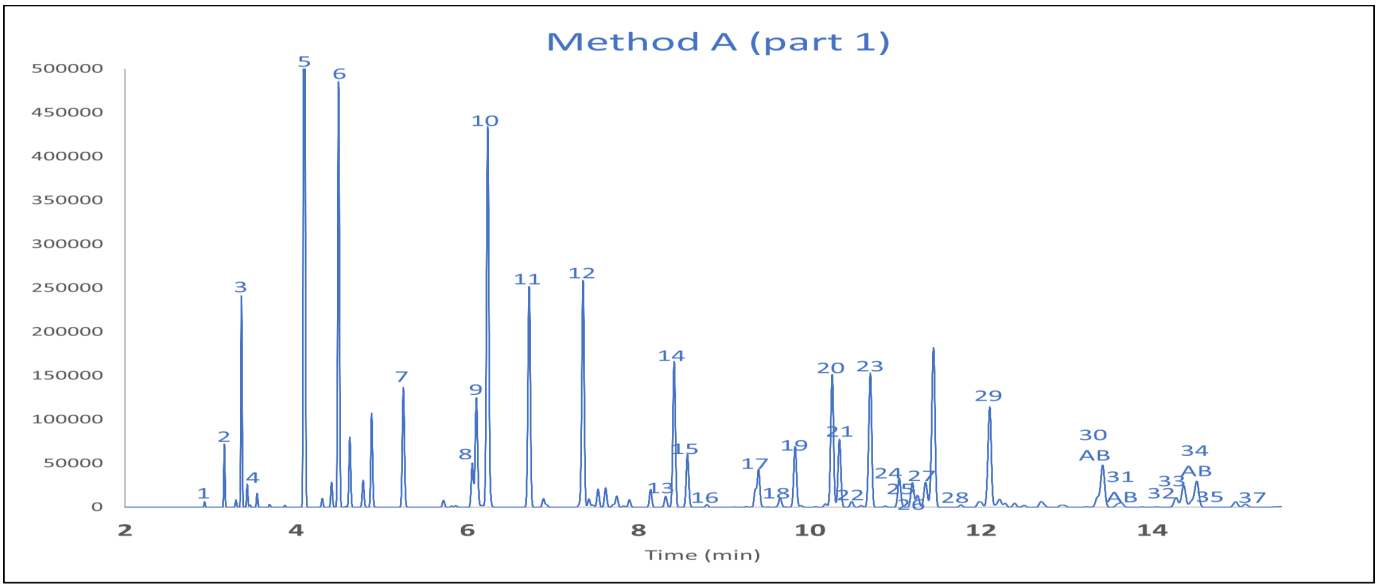
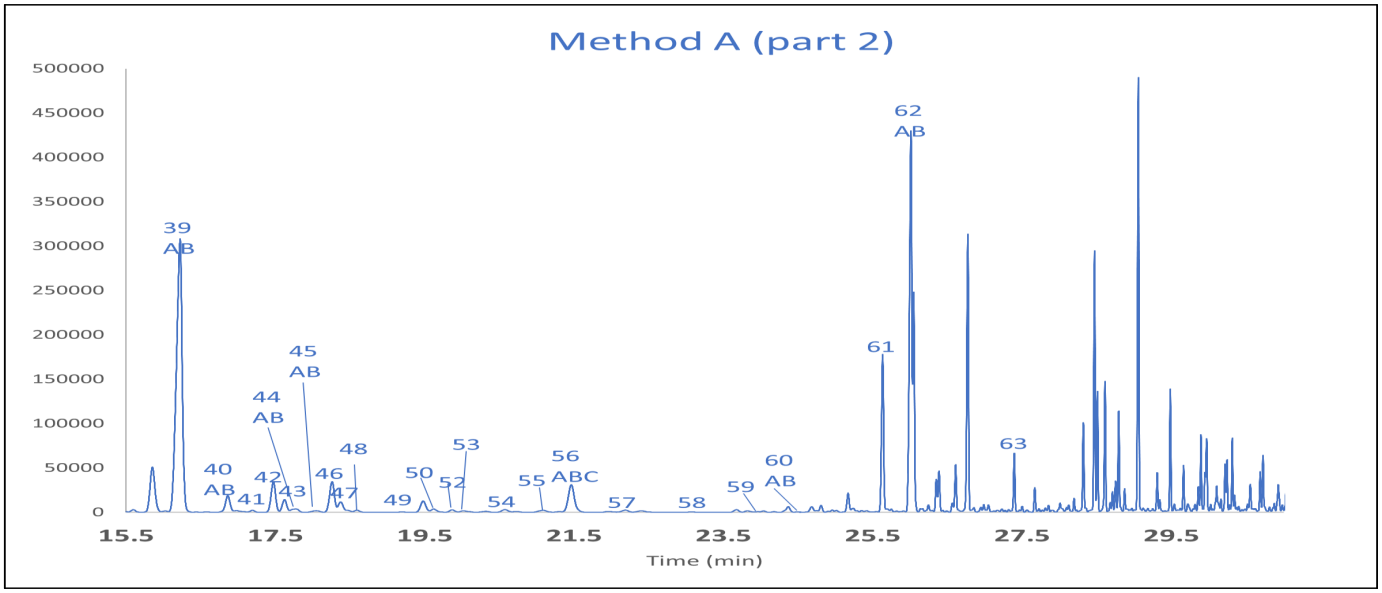
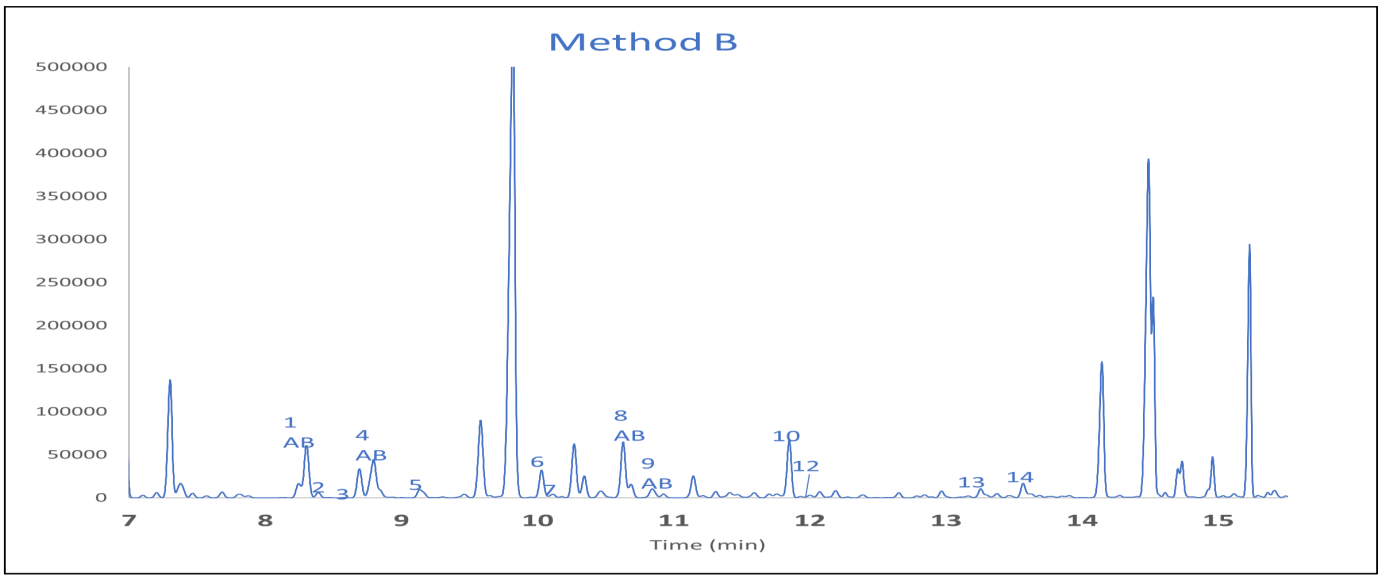
Figure 2. Example of a chromatogram of an gasoline standard using method A and method B.







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CONCLUSION

The Scion 4X6-GC analyser equipped with a split/ spitless injector, Scion Instruments column and FID is capable of performing UOP690 in a way that complies to the method.

The C_8 and low boiling paraffins and naphthenes are determined on the basis of mass-%, The quantitation limit for any reported component is 0.01 mass-%.

The equipment of the 4X6-GC analyser is pre determined, for ordering information or customisation, please contact your local sales representative.

SCION Instruments

UK
Livingston Business Centre
Kirkton South Road, Livingston
West Lothian EH54 7FA
Scotland, UK
Phone +44 1506 300 200
sales-eu@scioninstruments.com

The Netherlands
Amundsenweg 22-24
4462 GP Goes,
The Netherlands
Phone +31 (0) 113 287 600
sales-eu@scioninstruments.com