

Product Composition/Monitoring

Test Substance
 Category Name: GAS OILS CATEGORY

Category Chemical : Light Hydrocracked Gas Oil, CAS No. 64741-77-1

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Test Substance Purity/Composition and Other Test Substance Comments :

Density (ASTM D4052) @ 15°C/59°F 0.8244 g/mL
 Relative Density @ 60°F 0.8248 g/mL
 API Gravity @ 60°F..... 40.1 °API
 Boiling Range (ASTM D2887):
 initial..... 134.4 °C
 final..... 290.4 °C
 Hydrocarbon Types by FIA (ASTM D1319):
 Aromatics 16.7 vol %
 Olefins..... 1.5 vol %
 Saturates..... 81.8 vol %
 Determination of aromatic content by supercritical fluid chromatography (ASTM D5186):
 Monoaromatics 20.8 Wt %
 Polynuclear aromatics <0.5 Wt %
 Total aromatics..... 21.0 Wt %
 Above data from Intertek. 2009. Report of analysis, Reference no. US785-0017157. Intertek, Deer Park, Texas.

Reference : ExxonMobil Research and Engineering Co. 2010. Analysis report, Reference No. 2011AN 02. Annandale, NJ, USA.

Description :

The results field provides an attachment containing high resolution two dimensional gas chromatography (2D-GC) with flame ionization detection of a sample of light hydrocracked gas oil (CAS No. 64741-77-1). This sample was used in aquatic toxicity testing for complete data gaps for biodegradability, fish acute toxicity, invertebrate acute toxicity, invertebrate chronic toxicity, and algal toxicity.

GCxGC Chromatographic Conditions
 The sample was analyzed directly by GCxGC using the conditions shown below:
 Instrument: Agilent Technologies 6890 Series GC
 Injector: Split/Splitless in Split Mode
 Initial Temp 60°C
 Ramp 3°C/sec
 Final Temp 330°C
 Column flow at 1 mL/min in constant flow mode
 Split ratio at 1:50
 Sample injection: Agilent ALS- Injection volume 0.2 µL
 Modulator: Cryogenic modulator, single jet loop type (ZOEX Corporation)
 Modulation time 10 sec
 Pulse width 400 ms
 N2 Flow rate approx 5L/min, controlled by a flow meter
 Detector: Flame-ionization
 Temperature at 300°C
 Makeup gas He
 Makeup flow 20 mL/min

	<p>Hydrogen flow 40 mL/min Air flow 450 mL/min Column 1: 30 m x 0.25 mm i.d. 5% phenyldimethylpolysiloxane column (BPX-5) with film thickness of 1.0 µm Column 2: 3m x 0.25 mm i.d. polysilphenylene-siloxane column (BPX-50) with film thickness of 0.25 µm (One end of 2nd Dim column forms loop modulation, and the other end direct into FID) Carrier gas: Helium Oven temperature: 60°C (0 min isothermal) then 3.0°C/min to 240°C Hot Jet: 180°C offset from Oven: 240°C (0 min temperature isothermal) then 3.0°C/min to 390°C (50 min isothermal)</p> <p>Data Analysis GCxGC data is processed and visualized with in-house developed software.</p> <p>A mixture of normal paraffin from C10 to C28 has been used for qualitative analysis purpose to locate the retention position (both X-axis and Y-axis retention times) in the GCxGC. Based on the position of the normal paraffins; all other compound classes have been identified based on their relative position to normal paraffins.</p> <p>The peak area for each component or component group identified was directly integrated with the assumption of a universal unit response factor to all hydrocarbons by the flame ionization detector</p> <p>Having acquired the raw GCxGC data on the sample, the profile was examined and templates constructed to group individual components into the appropriate carbon number (C5 to C30) and chemical functionalities shown below:</p> <ul style="list-style-type: none"> • n-paraffins • iso-paraffins • n-alkane substituted cyclohexane and cyclopentane • mono-naphthenics • di-naphthenics • mono-aromatics • N-mono-aromatics • di-aromatics • N-di-aromatics • tri-aromatics • N-tri-aromatics • tetra-aromatics • N-tetra-aromatics • penta-aromatics
<p><u>Results:</u></p>	<p>Results are tabulated for the sample as shown in the spreadsheet. Numbers are reported in wt%. The peak area for each component or component group identified was directly integrated with the assumption of a universal unit response factor to all hydrocarbons by the flame ionization detector.</p> <p>The components found in the sample has been determined and tabulated in compound classes and carbon number order, as shown in the spreadsheet. The corresponding GCxGC chromatogram of the sample is also attached for reference</p>

purpose.

Please note the 2DGC method does not differentiate olefins from naphthenes.

2D-GC Analysis Results for light hydrocracked gas oil, CAS No. 64741-77-1.

C-num	nP	isoP	N	diN	triN	tetraN	pentaN		mono-A	N-mono-A	Di-A	N-Di-A	tri-A	N-tri-A	trtea-A	N-tetra-A	penta-A	
5	0.00								0									
6	0.00	0.00	0.00	0.00					0									
7	0.00	0.00	0.00	0.00					0.00									
8	0.01	0.00	0.83	0.00					0.19									
9	0.39	0.57	2.98	0.00					1.19	0.21								
10	0.87	1.50	6.79	6.70					1.86	2.10	0.00							
11	1.67	4.28	5.41	2.69					2.90	3.51	0.05							
12	1.77	4.74	4.95	1.66					2.09	2.25	0.12	0.00						
13	1.83	4.67	2.95	1.24					1.18	1.65	0.17	0.02						
14	2.31	3.90	1.86	0.67					0.56	0.54	0.11	0.02	0.00					
15	1.49	2.54	0.90	0.20					0.29	0.22	0.02	0.00	0.01					
16	0.63	1.25	0.22	0.02					0.07	0.04	0.01	0.01	0.01	0.05				
17	0.06	0.30	0.01	0.00					0.01	0.00	0.01	0.01	0.01	0.03	0.32			
18	0.00	0.01	0.00	0.00					0.00	0.02	0.01	0.01	0.01	0.02	0.21			
19	0.00	0.00	0.00	0.01					0.01	0.01	0.00	0.00	0.01	0.02	0.22	0.22		
20	0.00	0.00	0.01	0.00					0.00	0.00	0.00	0.01	0.01	0.01	0.14	0.35		
21	0.00	0.01	0.01	0.00					0.00	0.01	0.01	0.01	0.01	0.01	0.03	0.56		
22	0.00	0.02	0.00	0.00					0.00	0.00	0.01	0.01	0.01	0.01	0.01	0.59		
23	0.00	0.01	0.00	0.00	0.00	0.00			0.00	0.01	0.01	0.01	0.02	0.01	0.00			
24	0.00	0.01	0.00	0.00	0.00	0.00			0.01	0.01	0.01	0.01	0.02	0.01				
25	0.00	0.01	0.01	0.00	0.00	0.00			0.00	0.01	0.00	0.02	0.03	0.01				
26	0.00	0.01	0.01	0.00	0.00	0.00			0.00	0.01	0.02	0.02	0.02	0.00				
27	0.00	0.01	0.00	0.00	0.00	0.00			0.00	0.01	0.01	0.01	0.00					
28	0.00	0.01	0.00	0.00	0.00	0.00			0.00	0.02	0.01	0.00						
29	0.00	0.01	0.01	0.01	0.00	0.00			0.01	0.03								
30	0.01	0.01	0.01	0.01	0.00	0.00			0.01	0.03								
Total	11.06	23.89	26.98	13.24	0.02	0.02	0.00		10.39	10.69	0.58	0.16	0.16	0.18	0.92	1.72	0.00	100.00

Heading Codes:

C-num = number of carbon atoms in group; nP = normal paraffins; isoP = iso-paraffins; N = naphthenes; diN = di-naphthenes; triN = tri-naphthenes; tetraN = tetra-naphthenes; pentaN = penta-naphthenes; mono-A = monoaromatics; N-mono-A = naphthenic-mono-aromatics; Di-A = di-aromatics; N-Di-A = naphthenic-di-aromatics; tri-A = tria-aromatics; N-tri-A = naphthenic-tri-aromatics; tetra-A = tetra-aromatics; N-tetra-A = naphthenic-tetra-aromatics; penta-A = penta-aromatics.

2d-GC chromatogram of distillates (petroleum) light hydrocracked gas oil, CAS No. 64741-77-1

