

NORTH VIKING GRABEN GEOCHÉMICAL STUDY

GC-MS ANALYSIS

Well no. 30/6-3 NOCS

Client:

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The M/Z 205 fragmentogram shows a few peaks. The most prominent peaks are the $\beta\alpha$ homohopane (located between the $\alpha\beta$ homohopanes and the $\alpha\beta$ bishomohopanes) and the doublet representing the $\alpha\beta$ homohopanes. The M/Z 205 fragmentograms will show up the homohopanes strongly together with the demethylated hopanes, since the main fragmentation of the homohopanes gives a 191 and a 205 fragment. The other peaks in the fragmentogram are from the hopane and norhopane compounds. The very strong peaks from the $\alpha\beta$ homohopane again shows the sample to be relatively immature.

The molecular fragmentograms of the triterpanes show quite prominent peaks for the C_{28} , C_{29} , C_{30} and C_{31} triterpanes, while the C_{27} give a relative large noise to peak ratio, but the 17 α (H) trisnorhopane and the 18 α (H) trisnorneohopane can easily be distinguished.

Steranes:

When evaluating the steranes, all the various fragmentograms are compared. These show the 20S and 20R C₂₇ rearranged steranes to be the most prominent peaks together with 20R C₂₉ sterane. The general low abundance of steranes compared with the rearranged steranes is typical for samples of Upper Jurassic age in the Viking Graben. The very low abundance of the C₂₁ and C₂₂ steranes clearly shows that the sample is relatively immature.

Bicyclanes:

The M/z 123, 179 and 193 fragmentograms show a number of peaks in the bicyclane range, but are not very informative for this sample.



Aromatic Fraction

Thiophenes:

The M/Z 84, 98, 112, 126 and 140 fragmentations for thiophene and alkyl-substituted thiophenes also show a number of other peaks, which were not identified and are therefore difficult to evaluate.

The M/Z 84 fragmentogram shows a group of peaks with retention times between 23 and 27 minutes together with a large peak with a retention time of approximately 29 minutes. The M/Z 98 fragmentogram shows a large peak at the front of the fragmentogram together with a series of smaller peaks with a retention time between 18 and 36 minutes. The M/Z 112 fragmentogram shows a few peaks with very long retention times, (36 minutes and higher) while the M/Z 126 fragmentogram shows a similar series of peaks as in the M/Z 98 fragmentograms except for the front end peaks. These were probably present and have been lost during storage. The M/Z 140 fragmentograms show also the same peaks as in the M/Z 98 fragmentogram, but the peaks with shortest retention times have the largest abundance.

Alkyl-substituted Benzenes:

The alkyl-substituted benzenes are seen in the M/Z 106, 134 and 148 fragmentograms. There is a distinctive series of doublets for the M/Z 106 fragmentogram. The two other fragmentograms are not as distinctive. The M/Z 134 shows a prominent doublet at the front of the fragmentogram, while the C₄ alkyl-substituted benzenes are present only in trace amounts. The M/Z 148 shows a low signal to noise ratio, and a series of minor peaks.



Naphthalenes:

The M/Z 142 fragmentogram shows the typical doublet for the methyl-substituted naphthalenes, with an almost similar peak height for both 2-methyl- and 1-methylnaphthalenes. The M/Z 156 representing the C2-naphthalenes shows the 2+1-ethylnaphthalene peaks to be of almost the same height the 2,6 + 2,7 dimethylnaphthalene peaks, which as is slightly smaller than the 1,4 + 2,3 + 1,2 dimethyl-M/Z 170 fragmentogram shows naphthalene peak. The the pattern for C₂-naphthalenes. The peaks with longest retention times are particularly abundant in this sample.

Benzothiophenes and Dibenzothiophenes:

The various benzothiophenes and dibenzothiophenes are detected by M/Z 162, 176, 184, 198 and 212 fragmentograms. The M/Z 162 fragmentogram show a distinctive triplet where the middle peak is the largest. The M/Z 176 show a quartet for the C₂-substituted benzothiophenes, but the peaks are very small since the fragmentogram is dominated by one peak with a longer retention time. The M/Z 184 fragmentogram shows the single peak representing the dibenzothiophene, while the M/Z 198 shows the typical triplet for the methylsubstituted dibenzothiphenes. 1-methyldibenzothiophene i\$ the largest peak, which clearly indicates that the sample is immature. The large 1-methyldibenzothiophene compared with the other methyl-substituted dibenzothiophenes could also be due to a highly anoxic environment of deposition. The amount of C2-substituted dibenzothiophenes is relative low for this sample, which are also poorly resolved.

Phenanthrenes:

The M/Z 178 fragmentogram which would show the phenanthrene and anthracene if present, shows a large peak, identified as



phenanthrene and a smaller peak, approximately 10 % of the phenanthrene peak, identified as anthracene. The 192 M/Z fragmentogram shows the normal four peaks for the methylphenanthrenes. 3-methyl- and 2-methylphenanthrene are of approximately equal height. They are approximately 60 જ of the height of 9-methyl- and 1-methylphenanthrene. The M/Z 206 fragmentograms shows a low signal to noise ratio, indicating a low concentration of dimethyl-substituted phenanthrenes. Due to the low concentration it is difficult to make any evaluation of this fragmentogram. The M/Z 220 fragmentograms show a poor separation between the different peaks. The peaks with longest retention times have a higher relative abundance than is normally found.

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Aromatic Steranes:

The M/Z 253 fragmentogram shows a relatively good abundance of monoaromatic steranes. One of the C₂₉ peaks (H_{1}) is particular abundant sample. The in this M/Z 231 fragmentogram shows a large abundance of compounds with a below the C_{20} triaromatic steranes. retention time These peaks dominate the fragmentogram. The triaromatic components can still be seen and these show a normal distribution for an immature sample from the Viking Graben.



BRENT GROUP

Saturated Fraction

Terpanes:

The analysed sample from the Brent Gr. (2458 - 2461 m) shows, as for the sample from the Heather Fm. a number of peaks in the M/Z 163 fragmentogram representing steranes and triterpanes. The major peak found at an earlier retention time than the steranes and triterpanes. This peak, suspected to be Bis-(3-tert-buty1-5 ethy1-2 hydroxy pheny1) methane is probably an oxidizing agent from the septa on the sampling flasks. The sterane peaks have, on the whole a lower abundance compared with the triterpanes than was found in the Heather Fm. sample. The M/Z 177 fragmentogram shows that the $\alpha\beta$ and $\beta\alpha$ norhopanes are more prominent than in the Heather Fm. sample. The two peaks are again of approximately equal height, with the $\alpha\beta$ norhopane being slightly larger.

The M/Z 191 fragmentogram also contains the contaminant from septa. It has the same retention time as the the C₂₅ tricyclic terpanes and will, when present, qive distorted picture of the amount of these compounds. The fragmentogram shows a normal picture of the triterpanes with $\alpha\beta$ hopane as the most prominent peak. The triterpanes are much more prominent than the tricyclic terpanes, similar to that found in the Heather Fm. The T_{M}/T_{S} ratio is again very low. The most striking difference between this sample and the sample from the Heather Fm. is that the bisnorhopane peak is far smaller in this sample compared with the C_{27} and C₂₉ hopanes than what was found in the Heather Fm. sample. The various $\beta \alpha$ hopanes are again found to be prominent peaks indicating a low maturity. The 22R/22S ratio has approximately the same range for this sample as in the Heather Fm. sample, indicating a similar maturity. The



M/Z 205 fragmentogram shows the same peaks as found in the Heather Fm. sample. The main difference between the two samples is that the peak representing the $\alpha\beta$ hopane is relatively more prominent in the Brent Gr. sample compared with the Heather Fm. sample. The molecular fragmentograms for the Brent Gr. sample is similar to that found in the Heather Fm. sample, with exception of the M/Z 384. This clearly shows the lower abundance of bisnorhopane compared with the other pentacyclic triterpanes, compared with the Heather Fm. sample.

Steranes:

The various fragmentograms representing steranes show significant differences between the Brent Gr. sample and the sample from the Heather Fm. The M/Z 189 and 259 fragmentograms show that the C₂₇ rearranged steranes are less abundant compared with the C₂₉ rearranged steranes for the Brent Gr. sample than in the Heather Fm. sample. This is also seen for the normal steranes. The M/Z 217 shows the 20R-24-ethylcholestane to be almost of the same magnitude as 20R-βα-ethyldiacholestane, the while the and C27 C28 steranes are only slightly larger in the sample from the Brent Gr. compared with the sample from the Heather Fm. This change in the relative abundance of different rearranged and normal steranes, together with the increase in normal steranes compared with rearranged steranes indicate a different type of source, to one with a more terristrial origin. The abundance of C_{21} and C_{22} steranes appears to be larger in the sample from the Brent Gr. compared with the sample from the Heather Fm. This is a false impression, due to the height of the peaks when normalized to the largest peak, which in both instances is $20R-\beta\alpha$ -ethyldiacholestane. relative abundance Since the of rearranged steranes decreases compared with normal steranes, then the relative abundance of C_{21} and C_{22} steranes compared to $C_{27} - C_{28}$ regular steranes is approximately the same for the two

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samples. The fragmentograms of the different molecular ions of the steranes show basically the same as the rest of the sterane fragmentograms, i.e. an increase of the regular steranes relative to rearranged steranes for the Brent Gr. sample compared with the Heather Fm. sample.

Bicyclanes:

The M/Z 123, 179 and 193 show similar pattern as that found for the Heather Fm. sample.

Aromatic Fraction

Thiophenes:

fragmentograms for thiophene and The various alkylsubstituted thiophenes vary substantially compared with the sample from the Heather Fm.. The M/Z 84 fragmentogram shows again a series of peaks with retention time between 23 and 27 minutes. These peaks are very prominent in the sample from the Brent Gr., while they were minor compounds in the sample from the Heather Fm. The alkyl-substituted thiophenes also show large differences between the two samples, which probably represents differences in the organic matter of the two samples. The M/Z 98 fragmentogram shows the same peaks between 18 and 30 minutes in retention time for the two samples, while the peaks with retention times greater than 30 minutes are different. Two peaks are dominant in this section of the fragmentogram.

The M/Z 112 fragmentogram shows mainly one peak with retention time 42 minutes, while the M/Z 126 fragmentogram shows a similar distribution to the M/Z 98 fragmentogram, except that the front end peaks are absent. These may have been lost during storage. The M/Z 140 fragmentogram shows a



distribution similar to that at the front end of the M/Z 98 fragmentogram.

Alkyl-substituted Benzenes:

The alkyl-substituted benzenes show differences between the two samples in the M/Z 106 fragmentogram, while the rest of the fragmentograms are similar. The major difference in the M/Z 106 fragmentogram is a significant increase in the high molecular weight compounds as compared with the medium molecular weight compounds for the Brent Gr. samples compared with the Heather Fm. samples. This is believed to be due to a change in the type of organic matter.

Naphthalenes:

The M/Z 142 fragmentogram showing the methylnaphthalenes is similar to the one from the Heather Fm. sample, while the M/Z 156 fragmentogram, representing the C₂-naphthalenes shows a significant difference. The 1,6 and 1,3 + 1,7dimethylnaphthalenes are still the largest peaks with 2,6 + 2,7 and 1,4 + 2,3 and 1,5 peaks of approximately equal The relative height between the two peaks height. is reversed compared with the sample from the Heather Fm. The largest difference between the two samples is the relatively low intensity of the 2+1-ethylnaphthalenes and 1,2 dimethylnaphthalene in the sample from the Brent Gr. compared with the Heather Fm. The M/Z 170 fragmentogram show the typical pattern of peaks for C3-naphthalenes. The peaks with longest retention times have a lower relative abundance than found in the sample from the Heather Fm.

Benzothiophenes and Dibenzothiophenes:

The relative abundance of the C2-benzothiophenes seen in the



M/Z 162 fragmentogram changes in the sample from the Brent Gr. compared to the Heather Fm. sample. In the sample from the Brent Gr. the last peak in the triplet is the largest, while the middle peak is the largest in the sample from the Heather Fm. In the M/Z 176 fragmentogram, the quartet found for the sample from the Heather Fm. is not seen in the sample from the Brent Gr., which only shows one peak. The M/Z 184 fragmentogram again shows only the single peak from the dibenzothiophene, while the M/Z 198 fragmentogram shows the typical triplet for the methyl-substituted dibenzodistribution is distinctly different thiophenes. The from the sample from the Heather Fm. 4-methyldibenzothiophene is the largest peak and the 2+3-methyldibenzothiophene peak is approximately 40 % of this. 1-methyldibenzothiophene which was the largest peak in the sample from the Heather Fm. is the smallest peak in the sample from the Brent The Gr. C2-dibenzothiophenes show a group of six peaks in the M/Z separate 212 fragmentogram. The peaks were not identified, but peak 3 is the largest. Peaks 2 and 4 are approximately 80 % of the largest peak, while 5 is approximately 30 %. Peaks 1 and 6 are only minor.

Phenanthrenes:

The M/2 178 fragmentogram shows only one peak, phenanthrene. The small amount of anthracene seen in the sample from the Heather Fm. is not present in the sample from the Brent Gr, This could be due to an increased amount of phenanthrene ìn the sample with the result that the anthracene peak is less prominent or it could simply mean that anthracene is not present. The M/Z 192 fragmentogram representing the methylphenanthrenes is similar to that found in the sample from The M/Z 206 fragmentogram the Heather Fm.. shows some samples. The main difference differences between the two could be due to the low concentration of the C₂-phenanthrenes in the sample from the Heather Fm., making the peak height and the peak shape uncertain. The



 C_3 -phenanthrenes as seen by M/Z 220 give a series of peaks. They were not identified, but the distribution is significantly different from that seen in the sample from the Heather Fm.

Aromatic Steranes:

The monoaromatic steranes as seen by the M/Z 253 are difficult to identify and interprete. The $C_{27} - C_{29}$ monoaromatic steranes appear to be badly affected by other compounds coeluting with them and further interpretation is, therefore, not undertaken.

The M/Z 231 fragmentogram shows that the sample from the Brent Gr. has the same problems as the Heather Fm. sample with a large abundance of compounds before the C_{20} triaromatic steranes, making the aromatic compounds appear as minor peaks. Even so, a significant variation is seen both for the relative abundance of the C_{20} and C_{21} components, which is much larger for the Brent Gr. sample compared with the sample from the Heather Fm., and also in the C_{28} 20S component. This is much larger in the Brent Gr. sample than in the sample from the Heather Fm.

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DUNLIN GROUP

Saturated Fraction

Terpanes:

The M/Z 163 fragmentograms of the two samples from the Dunlin Gr. vary considerably. The sample from 2701 - 2788 m, which consists of the olive-grey, brown-grey claystone from the samples from 2701 - 2704 m and 2785 - 2788 m, have very low abundances of terpanes giving a low signal to noise ratio, making it impossible to distinguish the peaks. The sample from the 2809 - 2818 m, representing the olive-grey claystone from the Amundsen/Burton Fms. shows a good abundance of steranes and terpanes with the terpanes far more abundant than the steranes.

The M/Z 177 fragmentograms show similar features. The signal to noise ratio for the sample from 2701 - 2788 m is very low and the peaks are difficult to interprete, while the sample from 2809 - 2818 m has prominent peaks. This sample shows a peak eluting between 17 α trisnorhopane and bisnorhopane and is the second largest peak in the fragmentogram. This is believed to be a 17 β compound, but has not been identified. The presence of this compound shows the sample to be of low maturity, but it also shows that there is a difference in organic matter compared with the analysed samples from higher up in the well. The $\alpha\beta$ norhopane is the largest compound in the M/Z 177 fragmentogram for this sample, in clear opposition to the samples from the Heather Fm. and the Brent Gr., which either had equal abundance of the $\beta \alpha$ and $\alpha\beta$ norhopane or had the $\beta\alpha$ norhopane as the largest compound.

The M/Z 191 fragmentograms of the two samples differ significantly. The sample from 2701 m has a relative low

signal to noise ratio, but the C_{27} , C_{29} , C_{30} and C₃₁ triterpanes can be clearly distinguished. The contaminant peak coeluting with the C25 tricyclic terpane is clearly seen in the sample, which does not contain any tricyclic terpanes. The T_{S}^{T}/T_{M} ratio is low for this sample, similar to that found in samples higher up in the well. The sample does not contain any bisnorhopane and the most striking difference, compared with the samples from the the Brent Gr., is the Heather Fm. and relatively low abundance of $\alpha\beta$ hopane as compared with $\alpha\beta$ norhopane and 17 α trisnorhopane. This is clearly due to the difference in organic matter in this sample compared with the samples from the Heather Fm. and the Brent Gr.. The sample from 2809 -2818 m has a different M/Z 191 fragmentogram than the other analysed samples from this well. The difference between this sample and the sample from 2701 - 2788 m could be due to the low abundance of material in the latter, while the difference compared with the samples from the Heather Fm. and the Brent Gr. is real. The sample from 2809 - 2818 m shows a much larger abundance of both tricyclic and tetracyclic terpanes, than in the samples from the Heather Fm. and the Brent Gr.. In addition, the T_S/T_M ratio is much larger. This together with the large abundance of $\alpha\beta$ norhopane shows that the sample is quite different, and represents a different type of organic matter. The different maturity ratios indicate that this sample is slightly more mature than the samples from the Heather Fm. and Brent Gr.

The M/Z 205 fragmentograms of the two samples show that the sample from 2701 - 2788 m has a very low signal to noise ratio and the results are therefore difficult to interpret. The sample from 2809 - 2818 m shows a peak pattern which is similar to that in the samples from the Heather Fm. and the Brent Gr.. The molecular ion fragmentograms show basically the same features as discussed above. The signal to noise ratio for the sample from 2701 - 2788 m is very low and it is impossible to deduce anything from these fragmentograms, while the sample from 2809 - 2818 m gives excellent results.

The M/Z 370 clearly shows three peaks where the ${\rm T}_{\rm S}$ is nearly as large as the T_{M} . The third peak is at the same retention time as the one that had a large peak in the M/Z 177 fragmentogram. The M/Z 384 fragmentogram has one large peak, which is only found in minor quantities in other samples together with a series of smaller peaks where the $\alpha\beta$ norhopane peak is the largest. The large peak has the same retention time as the compound described in the M/Z 177 fragmentogram. The M/Z 384 as the molecular ion shows this peak to be a C₂₈ triterpane. The exact configuration is not known, but with the large abundance of this peak present in the sample from the Amundsen/Burton Fms. this could be used as a good correlation indicator. The rest of the molecular ion fragmentation show patterns that are normal for samples from the North Sea.

Steranes:

The M/Z 149 fragmentograms of the two samples are quite different. The sample from 2701 - 2788 m shows basically two peaks which could be contaminants, while the sample from 2809 - 2818 m show a distribution that is relatively similar to that found in the samples from the Heather Fm. and the Brent Gr. The M/Z 189 and 259 fragmentograms have very low signal to noise ratios in the sample from 2701 - 2788 m, making it impossible to interprete the data. The sample from 2809 - 2818 m has, however, a good signal to noise ratio. The pattern of rearranged steranes is quite different from the Brent Gr. sample, showing a far larger proportion of C₂₇ rearranged steranes as compared with the C₂₉ rearranged steranes, clearly showing the difference in organic input. Similar features are also seen for the M/Z 217 and 218 fragmentograms. These fragmentograms show that the relative abundance of C₂₇ regular steranes compared to C₂₉ regular steranes is higher in the sample from the Amundsen/Burton Fms. than was found in the Brent Gr. sample. The fragmentograms of the molecular ions of the steranes show



distinct differences between those from the Heather Fm., Brent Gr. and the Amundsen/Burton Fms.. The most distinct feature is the relative increase of regular steranes compared to rearranged steranes in the sample from the Amundsen/Burton Fms.. This is especially the case for the C_{28} compounds.

Bicyclanes:

The M/Z 123, 179 and 193 fragmentograms show a number of peaks. There are clearly differences between the various samples, but due to difficulties with identification of the different peaks, further discussion will not be undertaken.

Aromatic Fraction

Thiophenes:

The M/Z 84 fragmentograms show a series of peaks. The pattern is similar for the two samples and distinctly different to those found in the Heather Fm. and Brent Gr. samples. The group of peaks with retention times between 23 and 27 minutes is still present, but in the Dunlin Gr. samples a doublet with a retention time between 29 and 31 minutes is present. This is much less prominent than in the Brent Gr. sample and only the first of these is seen in the sample from the Heather Fm.

The M/Z 98 fragmentograms show only the peaks with longest retention times. Again, the pattern is similar for the two samples, but quite different when compared to the samples higher up in the well. The M/Z 112 fragmentograms show only the peaks with longest retention times. The two samples have similar patterns. A similar situation is found in the M/Z 126 and 140 fragmentograms.



Alkyl-substituted Benzenes:

The pattern of alkyl-substituted benzenes in the M/Z 106 is quite similar for the two samples and relatively similar to that found in the sample from the Brent Gr.. The M/Z 134 and 148 fragmentograms and especially the M/Z 134 fragmentogram, show the two samples from the Dunlin Gr. are quite different to those from the Heather Fm. and the Brent Gr.. The peaks in these may represent other compounds than normally found, which may give important information for correlation purposes.

Naphthalenes:

The doublet representing the methyl-substituted naphthalenes is small in both the samples from the Dunlin Gr.. This could be due to a loss of low molecular weight material during work up in the laboratory and the results are therefore not discussed any further. The M/Z 156 fragmentograms showing the C₂-substituted naphthalenes are quite different from those found in the Heather Fm. and Brent Gr. samples. The main difference is in the relative abundance of the 1,4 + 2,3 + 1,5 dimethylnaphthalene peak. In the sample from 2701 - 2788 m it is the second largest peak, being almost 60 % of the 1,3 + 1,7 + 1,6 dimethyl peak. In the sample from 2809 -2818 m it is even larger, being 80 % of the largest peak. In 1,2 this sample the dimethylnaphthalene has also significantly increased compared with the other peaks, and is 40% of the major peak. In the samples from Heather Fm. and Brent Gr. it was only 20 % and 10 %, respectively. The variation seen here would also be a good source of 170 information for correlation purposes. The M/Zfragmentograms of the two samples are almost identical. There is a marked decrease in the abundance of the peaks with shortest retention times compared to the samples from the Brent Gr. and Heather Fm. This could be due to a loss during sample preparation.



Benzothiophenes and Dibenzothiophenes:

The M/Z 162 fragmentogram shows a very low signal to noise ratio. The samples do not contain benzothiophene. The peaks seen in the Heather Fm. and Brent Gr. are not detected in the samples from the Dunlin Gr.. The M/Z 176 shows only one both the samples, similar to that found in peak for the sample from the Brent Gr.. A similar feature is also seen for M/Z 184 dibenzothiophene. The M/Z 198 fragmentogram representing methyldibenzothiophenes, shows the typical triplet in both the samples, with 4-methyldibenzothiophene the largest compound in both samples. The only difference between the two samples and the sample from the Brent Gr. is the relative abundance of the two other peaks. The relative abundance of the 2+3- and 1-methyldibenzothiophene is both maturity- and environment-dependant and therefore not as important for correlation purposes as those parameters discussed above. The M/Z 212 fragmentograms of the two similar to that found in the sample from samples are very the Brent Gr.

Phenanthrenes:

The M/Z 178 fragmentograms show only one peak representing phenanthrene, while the M/Z 192 fragmentograms show the two doublets of methyl-substituted phenanthrenes. These are similar to samples higher up in the well. The M/Z 206 fragmentograms of the two Dunlin Gr. samples are also similar to that found in the samples higher up in the well. The M/Z 220 fragmentograms show a poor resolution and are, therefore, not discussed any further.

Aromatic Steranes:

As with the samples from the Brent Gr., the samples from the Dunlin Gr. have a number of large peaks eluting together



with the monoaromatic steranes in the M/Z 253 fragmentograms. This make it impossible to evaluate these samples. The two samples from the Dunlin Gr. have the same peaks with a retention time lower than C_{20} triaromatic sterane. These compounds dominate the fragmentograms, but the triaromatic steranes can easily be detected. They show a pattern similar to that in the Heather Fm. samples.

Experimental, combined gas chromatography - mass spectrometry (GC-MS)

The GC-MS analyses were performed on a VG TS250 system interfaced to a Hewlett Packard 5890 gas chromatograph. The GC was fitted with a fused silica OV-1 capillary column (25m x 0.22 mm i.d.) directly into the ion source. Helium (10psi) was used as carrier gas and the injections were performed in splittless mode. The GC oven was programmed from 50°C to 150°C at 35°C/min. at which point the programme rate was 4° C/min up to 280° where the column was held isothermally for 37 min. For the aromatic hydrocarbons, the GC oven was programmed from 50oC to 280⁰C at 5°C/min. and held isothermally at 280 C for 22 min. The mass spectrometer was operated in electron impact (EI) mode at 70 eV electron energy, a trap current of 500 uA and a source temperature of 220°C. The instrument resolution was 2500 (10% valley) for most of the samples, but had to be decreased to 1000 for samples to improve the sensitivity of some some mass fragmentograms.

The datasystem used was a VG PDP11/73 system. The samples were analysed in multiple ion detection mode (MID) at a scan cycle time of approximately 1,8 sec.

Calculation of peak ratios was done from peak height in the appropriate mass fragmentograms.

In the discussion of the GC-MS data, the results will be discussed by area. The wells within an area will be discussed separately. In the discussion, samples within one formation are discussed together. The discussion is further divided into types of compounds as follows:

Saturated Fractions:

Terpanes:

The most commonly used fragmentions for detection of terpanes are M/Z 163 for detection of 25,28,30 trisnor-moretane or 25,28,30 trisnorhopane, M/Z 177 for detection of demethylated hopanes or moretanes, M/Z 191 for detection of tricyclic, tetracyclic- and pentacyclic terpanes and M/Z 205 for methylated hopanes or moretanes. The molecular ions M/Z 370, 384, 398, 412 and 426 are also recorded for identification of C_{27} , C_{28} , C_{29} , C_{30} and C_{31} triterpanes respectively.

Steranes:

The most commonly used fragmentions for detection of steranes are M/Z 149 to distinguish between 5 α and 5 β steranes, M/Z 189 and 259 for detection of rearranged steranes, M/Z 217 for detection of rearranged and normal steranes and M/Z 218 for detection of 14 β (H), 17 β (H) steranes. The molecular ions M/Z 372, 386, 400 and 414 are also recorded for identification of C₂₇, C₂₈, C₂₉ and C₃₀ steranes respectively.

Bicyclanes:

The fragmentions M/Z 123, 179 and 193 are normally used for



the detection of the bicyclanes (sesquiterpanes and diterpanes). M/Z 123 will detect all bicyclanes while M/Z 179 and 193 will show the C_{14} and C_{15} bicyclanes respectively.

Aromatic Fractions:

Alkyl-substituted Benzenes:

The M/Z 106 fragmentions is often used to detect the alkyl-substituted benzenes. It is especially useful for the detection of di-substituted benzenes. M/Z 134 can also be used for the C_A-alkylbenzenes, detection of but benzothiophene will also give a signal with this fragmention. M/Z 148 can be used for the detection of C₅-alkylbenzenes, but will give also signals for methyl-substituted benzothiophenes.

Naphthalenes:

Methylnaphthalenes are normally detected by the M/Z 142 fragmention while C_2 -naphthalenes are detected by M/Z 156 and C_3 -naphthalenes by M/Z 170.

Benzothiophenes and Dibenzothiophenes:

Benzothiophene can be detected, as mentioned above, by M/Z 134. The M/Z 198 and M/Z 212 fragmentions are used for methyl-substituted dibenzothiophenes and dimethyl-substituted dibenzothiophenes respectively.



Phenanthrenes:

Phenanthrene is detected using the M/Z 178 fragmention. Anthracene will, if present also give a signal in the M/Z 178 fragmention. Methyl-substituted phenanthrenes give signals in the M/Z 192 fragmention while the M/Z 206 fragmention shows the dimethyl-substituted phenanthrenes.

Aromatic Steranes:

Monoaromatic steranes are detected using the M/Z 253 fragmention while the triaromatic steranes are detected using the M/Z 231 fragmention.

2a. Mass Fragmentograms representing Terpanes

(M/Z 163, 177, 191, 205, 370, 384, 398, 412 and 426)

Peak identification. (α and β refer to hydrogen atoms at C-17 and C-21 respectively unless indicated otherwise).

Α.	18 α trisnorneohopane (T _S)	C ₂₇ H ₄₄	(I)
в.	17α trisnorhopane (T_{M})	C ₂₇ H ₄₆	(II, R=H)
z.	Bisnorhopane	C ₂₈ H ₄₈	(IV)
c.	αβ norhopane	C ₂₉ H ₅₀	$(II, R=C_2H_5)$
D.	βα norhopane	C ₂₉ H ₅₀	$(III, R=C_2H_5)$
Ε.	αβ hopane	C ₃₀ H ₅₂	$(II, R=i-C_3H_7)$
F.	βα hopane	C ₃₀ H ₅₂	$(III, R=i-C_3H_7)$
G.	22S αβ homohopane	C ₃₁ H ₅₄	$(II, R=i-C_4H_9)$
н.	22R αβ homohopane	C ₃₁ H ₅₄	$(II, R=i-C_4H_9)$
I.	$\beta \alpha$ homomoretane	^C 31 ^H 54	$(III, R=i-C_4H_9)$
J.	22S αβ bishomohopane	C ₃₂ H ₅₆	$(II, R=i-C_5H_{11})$
	22R $\alpha\beta$ bishomohopane	с ₃₂ н ₅₆	$(II, R=i-C_5H_{11})$
K.	22S αβ trishomohopane	C ₃₃ H ₅₈	$(II, R=i-C_6H_{13})$
	22R αβ trishomohopane	C ₃₃ H ₅₈	$(II, R=i-C_6H_{13})$
L.	22S αβ tetrakishomohopane	^C 34 ^H 60	$(II, R=i-C_7H_{15})$
	22R αβ tetrakishomohopane	C ₃₄ H ₆₀	$(II, R=i-C_7H_{15})$
М.	22S αβ pentakishomohopane	C ₃₅ H ₆₂	$(II, R=i-C_8H_{17})$
	22R αβ pentakishomohopane	C ₃₅ H ₆₂	$(II, R=i-C_8H_{17})$
P.	Tricyclic terpane	C ₂₃ H ₄₂	$(V, R=i-C_4H_9)$
Q.	Tricyclic terpane	$C_{24}H_{44}$	$(V, R=i-C_{5}H_{11})$
R.	Tricyclic terpane (17R, 17S)	C ₂₅ H ₆₆	$(V, R=i-C_6H_{13})$
s.	Tetracyclic terpane	$C_{24}H_{42}$	(VI)
т.	Tricyclic terpane (17R, 17S)	C ₂₆ H ₄₈	$(V, R=i-C_7H_{15})$
Ν.	Tricyclic terpane	C ₂₁ H ₃₈	$(V, R=C_2H_5)$
ο.	Tricyclic terpane	C ₂₂ H ₄₀	$(V, R=C_{3}H_{7})$
Υ.	25,28,30 trisnorhopane/moretane	C ₂₇ H ₄₆	(VII)
x.	Unknown triterpane	C ₃₀ H ₅₂	



STRUCTURES REPRESENTING TERPANES

















2b. <u>Mass Fragmentograms representing Steranes</u>

(M/Z 149, 189, 217, 218, 259, 372, 386, 400 and 414)

Peak identifications. (α and β refer to hydrogen atoms at C-5, C-14 and C-17 in regular steranes and at C-13 and C-17 in diasteranes).

a.	205 βα diacholestane	$C_{27}H_{48}$	(I,	R=H)
b.	20R βα diacholestane	C ₂₇ H ₄₈	(I,	R=H)
с.	20S αβ diacholestane	C ₂₇ H ₄₈	(II,	R=H)
d.	20R αβ diacholestane	C ₂₇ H ₄₈	(II,	R=H)
e.	20S $\beta \alpha$ 24 methyldiacholestane	C ₂₈ H ₅₀	(I,	R=CH ₃)
f.	20R $\beta\alpha$ 24 methyldiacholestane	C ₂₈ H ₅₀	(I,	$R=CH_3$)
g.	20S $\alpha\beta$ 24 methyldiacholestane	C ₂₈ H ₅₀	(II,	$R=CH_3$)
	+ 20S ααα cholestane	C ₂₇ H ₄₈	(III,	R=H)
h.	20S $\beta \alpha$ 24 ethyldiacholestane	C ₂₉ H ₅₂	(II,	$R=C_2H_5$)
	+20R αββ cholestane	C ₂₇ H ₄₈	(IV,	R=H)
i.	20S αββ cholestane	C ₂₇ H ₄₈	(IV,	R=H)
	+20R $\alpha\beta$ 24 methyldiacholestane	C28 ^H 50	(II,	R=CH ₃)
j.	20R ααα cholestane	C ₂₇ H ₄₈	(III,	R=H)
k.	20R $\beta \alpha$ 24 ethyldiacholestane	C ₂₉ H ₅₂	(I,	$R=C_{2}H_{5}$)
1.	20S $\alpha\beta$ 24 ethyldiacholestane	C ₂₉ H ₅₂	(II,	$R = C_2 H_5$)
m.	20S ααα 24 methylcholestane	^C 28 ^H 50	(III,	$R=CH_3$)
n.	20R $\alpha\beta\beta$ 24 methylcholestane	^C 28 ^H 50	(IV,	R=CH ₃)
	+ 20R $\alpha\beta$ 24 ethyldiacholestane	C ₂₉ H ₅₂	(II,	$R = C_2 H_5$)
ο.	20S $\alpha\beta\beta$ 24 methylcholestane	C28 ^H 50	(IV,	R=CH ₃)
p.	20R aaa 24 methylcholestane	^C 28 ^H 50	(III,	R=CH ₃)
q.	20S $\alpha\alpha\alpha$ 24 ethylcholestane	C ₂₉ H ₅₂	(III,	$R = C_2 H_5$)
r.	20R $\alpha\beta\beta$ 24 ethylcholestane	C ₂₉ H ₅₂	(IV,	$R = C_2 H_5$)
s.	20S $\alpha\beta\beta$ 24 ethylcholestane	C ₂₉ H ₅₂	(IV,	$R=C_2H_5$)
t.	20R ααα 24 ethylcholestane	C ₂₉ H ₅₂	(III,	$R = C_2 H_5$)
u.	5 α sterane	C ₂₁ H ₃₆	(VI,	$R=C_2H_5$)
v.	5α sterane	C ₂₂ H ₃₈	(VI,	R=C3H7)



STRUCTURES REPRESENTING STERANES















Mass Fragmentograms representing Triaromatic Steranes (M/Z 231)

Description of ABC-ring triaromatic steroid hydrocarbons

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	Substitu	ents	Abbreviation		
Peak	R ₁	^R 2	of Compound		
a1	CH3	Н	C ₂₀ TA		
b1	Сн ₃	CH3	C ₂₁ TA		
c1	S(CH ₃)	C ₆ H ₁₃	SC ₂₆ TA		
d1	R(CH ₃)	C ₆ H ₁₃	RC ₂₆ TA		
	S(CH ₃)	C ₇ H ₁₅	SC ₂₇ TA		
el	S(CH ₃)	C ₈ H ₁₇	SC28TA		
fl	S(CH ₃)	C7H15	RC ₂₇ TA		
g1	R(CH ₃)	C ₈ H ₁₇	RC ₂₈ TA		



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STRUCTURES REPRESENTING TRIAROMATIC STERANES:









Mass Fragmentograms representing Monoaromatic Steranes (M/Z 253)

Description of C-ring monoaromatic steroid hydrocarbons

		Substit	Abbreviation		
Peak	R ₁	R ₂	R ₃	R ₄	of Compound

A1					C ₂₁ MA
В1	an a	a uu			C ₂₂ MA
C1	<u> β(H)</u>	CH ₃	S(CH ₃)	Н	βSC ₂₇ MA
	CH3	H	S(CH ₃)	H	SC ₂₇ DMA
	β(H)	CH3	R(CH ₃)	Н	βRC ₂₇ MA
D1	CH3	H	r(CH ₃)	Н	rc ₂₇ dma
	α(Η)	CH ₃	S(CH ₃)	н	αsc ₂₇ ma
E1	β(Η)	CH3	S(CH ₃)	CH3	βsc ₂₈ ma
	CH3	H	s(CH ₃)	CH ₃	SC ₂₈ DMA
F1	_α (Η)	СН3	R(CH ₃)	H	arc ₂₇ MA
	$\alpha(H)$	CH3	S(CH ₃)	CH3	asc ₂₈ ma
	β(H)	CH3	R(CH ₃)	CH3	BRC28MA
G1	CH3	H	R(CH ₃)	CH3	RC ₂₈ DMA
	β(Н)	CH3	S(CH ₃)	с ₂ н ₅	βsc ₂₉ ma
	CH3	H	S(CH ₃)	^с 2 ^н 5	sc ₂₉ dma
	α(H)	CH3	R(CH ₃)	CH3	arc ₂₈ MA
Hl	β(н)	СН3	R(CH ₃)	с ₂ н ₅	BRC ₂₉ MA
	CH3	H	R(CH ₃)	с ₂ н ₅	rc ₂₉ dma
11	α(H)	CH3	R(CH ₃)	C2H5	a RC ₂₉ MA



STRUCTURES REPRESENTING MONOAROMATIC STERANES:





Table 1: Variation in Triterpane Distribution for Well NOCS 30/6-3

Depth unit of measure: m

				В									C+D		J1	
Depth	Lithology	B/A	B/B+A	B+E+F	C/E	C/C+E	X/E	Z/E	Z/C	Z/Z+E	Q/E	E/E+F	C+D+E+F	D+F/C+E	J1+J2%	Sample
2410.00	bulk	5.07	0.84	0.22	0.51	0.34	0.06	0.34	0.66	0.25	0.02	0.83	0.36	0.25	50.49	117-0
2473.00	bulk	5.88	0.85	0.25	0.49	0.33	0.03	0.13	0.27	0.12	0.02	0.83	0.35	0.25	54.23	118-0
2788.00	bulk	4.84	0.83	0.31	0.70	0.41	-	-	-	-		0.80	0.42	0.26	63.46	120-0
2818.00	bulk	2.12	0.68	0.30	0.79	0.44	0.04	0.11	0.14	0.10	0.06	0.82	0.45	0.22	57.39	121-0



Table 2: Variation in Sterane Distribution for Well NOCS 30/6-3

Depth unit of measure: m

Depth	Lithology	Ratiol	Ratio2	Ratio3	Ratio4	Ratio5	Ratio6	Ratio7	Sample
2410.00	bulk	0.60	21.75	61.91	0.61	0.79	0.09	0.07	1 17–0
2473.00	bulk	0.58	23.30	56.10	0.38	0.73	0.16	0.13	118-0
2788.00	bulk	-	-						120-0
2818.00	bulk	0.37	76.94	73.49	0.50	0.64	0.23	0.16	121-0

Ratiol: a / a + j		Ratio5: r	+ s /	r +	s +	q							
Ratio2: $q / q + t * 1$.00%	Ratio6: u	+ v /	u +	v +	q +	r +	s -	⊦ t				
Ratio3: $2(r + s)/(q + s)$	· t + 2(r + s)) * 100%	Ratio7: u	+ v /	u +	V +	ì +	m +	n -	ŀq	+	r +	S ·	+t
Ratio4: $a + b + c + d$	l/h+k+l+n												



Table 3: Aromatisation of Steranes for Well NOCS 30/6-3

Depth unit of measure: m

Depth	Lithology	Ratio1	Ratio2	Sample
2410.00	bulk	0.72	0.67	117-0
2473.00	bulk	0.80	0.59	118-0
2788.00	bulk	0.58	0.70	120-0
2818.00	bulk	0.70	0.52	121-0

Ratiol: C1+D1+E1+F1+G1+H1+I1

Ratio2: g1 / g1 + I1

Cl+Dl+El+Fl+Gl+Hl+I1 + cl+dl+el+fl+gl



Table 4: Variation in Triaromatic Sterane Distribution for Well NOCS 30/6-3

Depth unit of measure: m

Depth	Lithology	Ratiol	Ratio2	Ratio3	Ratio4	Ratio5	Sample
2410.00	bulk	0.50	0.44	0.23	0.24	0.33	117-0
2473.00	bulk	0.73	0.71	0.51	0.47	0.66	118-0
2788.00	bulk	0.50	0.43	0.19	0.23	0.28	120-0
2818.00	bulk	0.77	0.67	0.33	0.46	0.43	121-0

 Ratio1: al / al + gl
 Ratio2: al / al + el + fl + gl

 Ratio2: bl / bl + gl
 Ratio5: al / al + dl

 Ratio3: al + bl / al + bl + cl + dl + el + fl + gl



Table 5: Variation in Monoaromatic Sterane Distribution for Well NOCS 30/6-3

Depth unit of measure: m

Depth	Lithology	Ratio1	Ratio2	Ratio3	Ratio4	Sample
2410.00	bulk	0.20	0.14	0.12	0.09	117-0
2473.00	bulk	0.30	0.22	0.12	0.09	118-0
2788.00	bulk	0.30	0.22	0.15	0.14	120-0
2818.00	bulk	0.27	0.19	0.14	0.11	121-0

Ratio1: A1 / A1 + E1 Ratio2: B1 / B1 + E1 Ratio3: A1 / A1 + E1 + G1 Ratio4: A1+B1 / A1+B1+C1+D1+E1+F1+G1+H1+I1

