C1-C31 analysis data can be used to obtain the same information as that obtained from C12+ GC but further provides detailed compositional data on the C1-C11 fraction and enables calculation of the distillation range of the sample.

13. MOLECULAR SIEVE EXTRACTION

This technique is used to isolate the branched/cyclic alkanes from the saturate fraction for gas chromatography/mass spectometry analysis. A mixture of saturates: 5A molecular sieves: purified benzene in the proportions 1:5:12 by weight is placed in a 100ml round bottom flask and refluxed for 24 hours. After cooling, the seives are filtered from the liquid phase and are washed with 4 x 10ml aliquots of benzene. The liquid phase plus washing are freed of benzene by distillation yielding the branched/cyclic compounds.

14. COMPUTERIZED GAS CHROMATOGRAPHY/MASS SPECTOMETRY (GC/MS)

Gas chromatography/mass spectrometry employs a capillary column gas chromatograph linked in series with a mass spectrometer and data system (GC/MS/DS). As molecules are eluted from the capillary column they are bled into the analyser tube of the mass spectrometer where they are bombarded with high energy electrons and consequently fragment to form several ions each with molecular weights less than that of the parent molecule. The fragmentation pattern is characteristic of the particular molecular type. The spectrum of these ions (referred to as a mass spectrum) is recorded approximately once every second and all of the mass spectra recorded during a GC/MS/DS analysis are memorised by the data system. Since any given class of molecules will breakdown in the analyser type to give one or more characteristic ion fragments of known molecular weight, after a GC/MS/DS analysis it is possible to examine the distribution of compounds within a given class by having the data system reproduce a mass fragmentogram (plot of ion concentration against gas chromatography retention time) representative of the particular class.

GC/MS/DS analyses can be carried out using one of the two following modes of operation:

(i) Acquire mode - in which all ions in each mass spectrum are memorised by the data system;

(ii) Selective ion monitoring (SIM) mode - in which only selected ions of interest are memorised by the data system.

At present the sterane/triterpane/bicyclane fraction of petroleum is considered most useful for GC/MS/DS analysis and therefore we commonly use the second of the above mentioned modes of operation and run the following twenty-two ions which are pertinent to the sterane/triterpane/bicuclane fraction.

Ion	Molecular Type
177	Demethylated triterpanes
191	Normal triterpanes
205	Methyl triterpanes
163	Specific dethylated triterpanes
356	Parent ion - C26 triterpanes
370	Parent ion - C27 triterpanes
384	Parent ion - C28 triterpanes
398	Parent ion - C29 triterpanes