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THE OCCURRENCE OF ALKYLCYCLOPENTANES IN TORBANITES

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Monocyclic alkanes, which include alkylcyclopentanes, have been known to occur in oils and sediments since the mid 1900's (Petrov, 1984). The lower molecular weight monocyclic alkanes have been studied in detail in sediments (Hoffmann, 1987) and oils (George *et al.*, 2002). However, the reporting of the occurrence of higher molecular weight alkylcyclopentanes ($>C_{15}$) has been very infrequent (Shimoyama and Yabuta, 2002). This study sets out to positively identify some high molecular weight alkylcyclopentanes in torbanites.

Conventional quadropole GC-MS has been the method of choice for the analysis of a wide range of compounds, including monocyclic alkanes, however this method limits the sensitivity of analysis for high molecular weight alkylcyclopentanes due to their low concentration in a highly complex hydrocarbon matrix. For this reason, the mass spectrometer used in this study was operated in Multiple Reaction Monitoring (MRM) mode. This mode afforded ease of use coupled with a high degree of sensitivity.

In order to investigate the occurrence and analysis of these higher molecular weight alkylcyclopentanes in sediments, two C_{24} alkylcyclopentane standards were synthesised (2-methyl-octadecylcyclopentane and 3-methyl-octadecylcyclopentane) and analysed by GC-MS (MRM) to determine the best multiple transitions to use in the analyses of the samples.

Using GC analysis on the prepared standards, the elution order on a typical GC phase (DB-5) was determined and the *cis-*/*trans-* isomers of 2-methyl-octadecylcyclopentane were assigned using the elution order of *cis-*/*trans-* alkyl-2-methylcyclopentanes reported by Hughey *et al*. (2004). Multiple Reaction Monitoring analysis was then performed using selected transitions, the most abundant transition being m/z 336 → 308. This transition has been attributed to loss of C_2 from the cyclopentane ring.

A series of six Torbanite extracts, previously described and prepared by Audino *et al*. (2001), were analysed using the GC-MS setup as mentioned in the previous paragraph. In order to positively identify the alkylcyclopentanes, a previously analysed extract was "spiked" with the reference standards and re-run under the same conditions. The increase in the m/z 336 → 308 transition at the same retention time shows positive identification of the 2-methyl-octadecylcyclopentane and 3-methyl-octadecylcyclopentane (See Figure 1).

The results show that the occurrence of alkylcyclopentane is ubiquitous in the Torbanite extracts. Furthermore, using retention time comparison, there is excellent evidence that there is a homologous series of the alkylcyclopentane compounds. This includes the *cis* and *trans*- alkyl-2-methylcyclopentanes, *cis*- alkyl-3-methylcyclopenatnes and alkylcyclopentanes.

This is the first time that these high molecular weight alkylcyclopentanes have been positively identified in sediments.

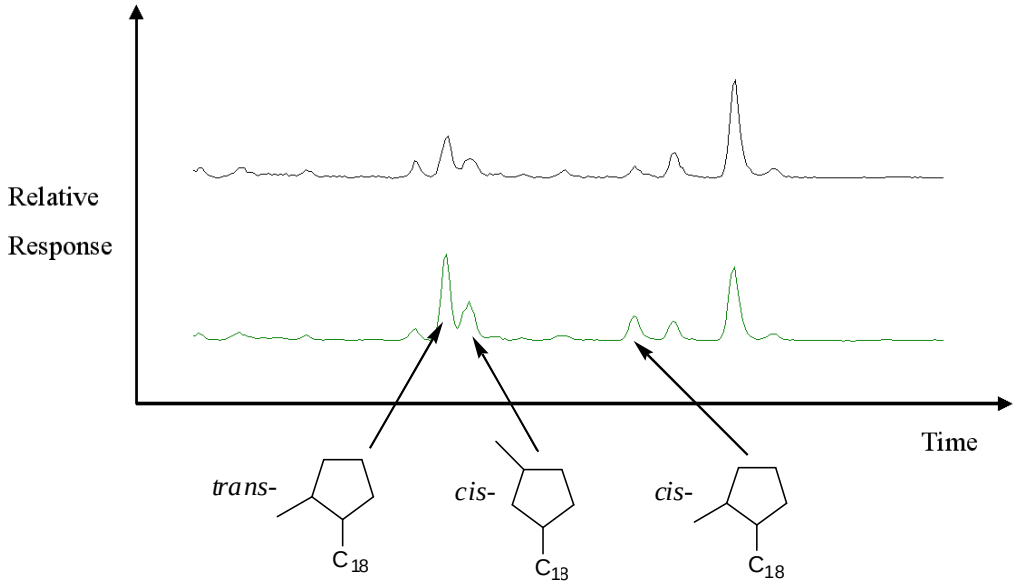

Figure 1. Top - MRM chromatogram (m/z 336 → 308) of a Permian Torbanite extract and Below - MRM analysis of the same extract spiked with reference alkylcyclopentane standards

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