Identification of decamethyl henicosane-products from c1´-2-3-2´ condensation of isoprenoids

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Introduction

The first identification of the HBI alkanes in the Maoming oil shale[1] was actually based on a comparison with the mass spectrum of C_{20} Highly branched isoprenoids (HBI)[2] from Rozel Point crude oil. However, the structural speculation seemed unsolid and thus under suspicious because not only their mass spectrum but also their co-chromatography results were both not identical to the later synthesized C_{30} HBI standard compound[3]. In addition, the source attribution of diatoms indicated by C_{30} HBIs was inconsistent with the sample. Thus, we purified the same HBI alkanes and structurally characterized them by MS and NMR.

Results and discussion

Two novel stereisomers decamethyl henicosanes ($C_{31}H_{64}$) (DMHs) (Fig. 1a, 1b) could be yielded by NMR and MS results, which completely different from that of previously speculated C_{30}-HBIs (Fig. 1c). A c1´-2-3-2´condensation[4] (cyclobutane ring) of two FPPs (farnesol diphosphates) and a subsequent fission of the c1´-2´ bonds, followed by methylation and geochemical hydrogenation is proposed to explain the geochemical presence of the novel polymethylhenicosanes in oil shale (Fig. 2).

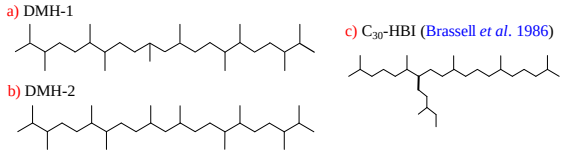

Figure 1: Comparison of novel DMHs and C_{30} HBI

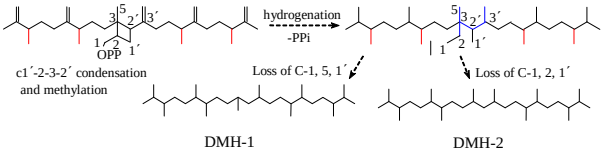

Figure 2: Possible precursors and pathway for the DMHs.

[1] Brassell *et al.* (1986) *Org. Geochem* **10**, 927-941. [2] Yon *et al.* (1982) *Tetrahedron Lett*. **23**, 2143-2146. [3] Rowland & Robson (1990) *Mar. Environ. Res* **30**, 191-216. [4] Thulasiram *et al*. (2007) *science* **316**, 73-76.