Tentative structural assignment for a new C_{33} botryococcane occurring in a Chinese Maoming sediment

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Introduction

An unknown compound (peak * in figure 1a) with gas chromatographic behavior resembling those for the C_{31}-C_{33} botryococcanes has been isolated from a Chinese Maoming sediment. EIMS (electron impact mass spectrometry) analysis was conducted for its probable structure.

Results and discussion

EIMS analysis of this compound showed the presence of, in addition to the fragment ions m/z 462 [M-2H]+ and m/z 434 [M-28-2H]+ characteristics of C_{33} botryococcanes[1], two unusual and unexpected key ions of m/z 224 and 238 but not 238 and 280 indicative of C_{33} botryococcanes. we suspect this compound is an isomer of the C_{33} botryococcane with a methyl α to the quaternary carbon which is reasonable for *m/z* 224 (figure 1b).

To the best of our knowledge, this is the first report of a new C_{33} botryococcane isormer in geological samples. Moreover, the novel *o*-methyl structure might indicate a new biosythethic pathway for its formation.

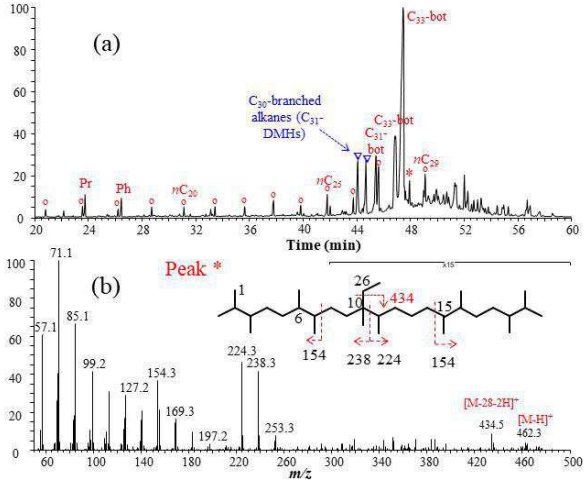

Figure 1: Comparison of novel DMHs and C_{30} HBI

[1] Brassell *et al.* (1986) *Org. Geochem* **10**, 927-941.