The theoretical estimation of mass-dependent fractionation line (MDFL) positions of oxygen isotopes

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Small mass-independent processes have been paid more and more attentions as potential new proxies of environment change. Angert *et al.* (2004) proposed that ^{17}O-excess in ice could indicate the variations in oceanic humidity and was confirmed by Landais *et al.* (2008). This kind of small mass-independent process studies require not only high precision analytical techniques, but also a high precision MDFL slope position in terms of λ values (i.e. 0.528 vs. 0.52) and the temperature dependence of λ. Here, we study the λ values of many important O isotope systems and try to establish a simple way of estimating unknown λ value if it is needed.

Based on the logarithm-type expression for small delta (δ), we calculated many λ' values by using high-level quantum chemistry methods. We find: 1) although anharmonicity affects the reduced partition function ratios (RPFR) for some molecules, it has little effect on the MDFL position due to large cancelation. 2) Crossover relates to the frequencies shifts (i.e. Δω) and also the frequencies shift factors (i.e. Δω/ω). Crossover usually occurs at relative low temperatures. 3) The λ' values are varied at different temperatures but are almost constant within a small temperature range, such as from -50°C to 50°C, which is a temperature range many studies focused on. 4) Because the number of actual λ' values is numerous, the work of producing these λ' values will be extremely demanding. Alternatively, we propose a simple way to predict the λ' values approximately. We find that the difference of λ' values between similar chemical structure units is small (often to the fourth digit after zero point). This finding enable us to estimate almost all λ' values if we have provided the beta values of the most typical O isotope systems.

[1] Angert *et al.* (2004) *GCA*, **68**, 3487–3495. [2] Landais *et al.* (2008) *GeoPhys. Res. Lett.* **35**, L02709.

Oil sources analysis in Northern Qaidam Basin, China

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Three GC/MS analyzed oil-bearing sand core samples whose depths were 135m, 158m and 319m respectively, all produced from Middle Jurassic in Mahaigaxiu anticline of Northern Qaidam Basin in China, show interesting different biomarker features. The two samples from shallower layer are mature oil and contain lacustrine and terrigenous organic matter preserved under oxic conditions. The sample from the deepest layer indicates lacustrine organic matter preserved suboxic and higher salinity conditions and is the only one which underwent biodegradation and immature oil. Oil-oil correlation between the three samples and other oil samples from surrounding area Yuqia and Mabei oil field indicates that the samples from shallower and deeper layers have very similar biomarker features with Yuqia oil and Mabei oil, respectively. Based on oil-oil correlation and thermal history analysis of source rocks, we consider that the mature oil in shallower layer came from the Middle Jurassic source rock in Yuqia depression which reached and maintained in the oil window in the early Cretaceous and the immature oil in the deeper layer migrated from the Middle Jurassic source rock in Gaxi depression which subsided in connection with the tectonic movement in Paleogene and reached the oil window and oil generation peak in late Paleogene..

With the help of seismic cross section analysis, fission track dating evidences and modelled time-temperature thermal history, we consider that this interesting event of immature oil and mature oil accumulated in deeper and shallower layers respectively was closely bound up with two tectonic movements in Cenozoic. In Paleogene, the immature oil from Yuqia depression migrated to Mahaigaxiu anticline which was formed by compression from South Qilian Mountains in the same period. In Neogene, the eastern end of mahaigaxiu anticline upwarped and the western end pitched because of the uplift of Lvliang Mountain which located in the western end of Mahaigaxiu. In the same period, many NE strike slip faults were formed and cut the Mahaigaxiu anticline. Mature oil from Gaxi depression migrated to the eastern end of the anticline and migrated vertically to the shallower layer when the oil met cutting faults.