An improved molecular sieve method for CSIA of *n*-alkanes

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Long-chain *n*-alkanes have been widelv employed as well-known biomarkers for exploring terrestrial vegetation in environmental studies. Their stable hydrogen and carbon isotope ratios (δD and δ^{13} C) have also been used to trace the delivery of terrestrial organic matter to aquatic environments and reconstruct the climate change in to paleoenvironments. For compound-specific isotope analysis, however, we must purify n-alkanes preserved in soils, sediments, or sedimentary rocks, from branched/cyclic hydrocarbons and UCM (unresolved complex mixture) in the samples.

Several conventional purification methods including molecular sieve and urea adduction were established for the isotope analysis. Molecular sieve method has been recognized to achieve high purify with physical mesh size separation. However, this procedure includes a great risk on the use of hydrofluoric acid (HF), which is very toxic and hazardous to our health. Therefore, many organic geochemists don't like the use of molecular sieve method for *n*-alkane purification.

In this study, we demonstrated a safer molecular sieve method for the *n*-alkane purification from branched hydrocarbons (e.g., pristane). *n*-Alkanes, which are trapped in the multi-holes of molecular sieve, are released by digestion of the molecular sieve cage with HF. As a new procedure, the hydrofluoric acid is then completely neutralized with sodium hydroxide (NaOH) to form sodium fluoride (NaF) and subsequently with calcium chloride (CaCl₂) to precipitate fluorine as stable particles (CaF₂). *n*-Alkanes are then extracted easily and safety with *n*hexane from the neutralized aquatic layer.

In the improved method, *n*-alkanes are quantitatively separated from pristane, and their hydrogen and carbon isotopic compositions are identical with known values within 10% and 0.5%, respectively. The improved method thus will be a safer method for the preparation and measurement of *n*-alkane isotope ratios. In the presentation, we would like to show details of the improved method, with the observed isotope data for the isotopic reference *n*-alkanes and for *n*-alkanes in natural samples.