Isotomics

Fall 2015

What we do

Isotomics develops and uses cutting-edge analytical techniques to understand the patterns of abundance and distribution of isotopes in natural molecules.

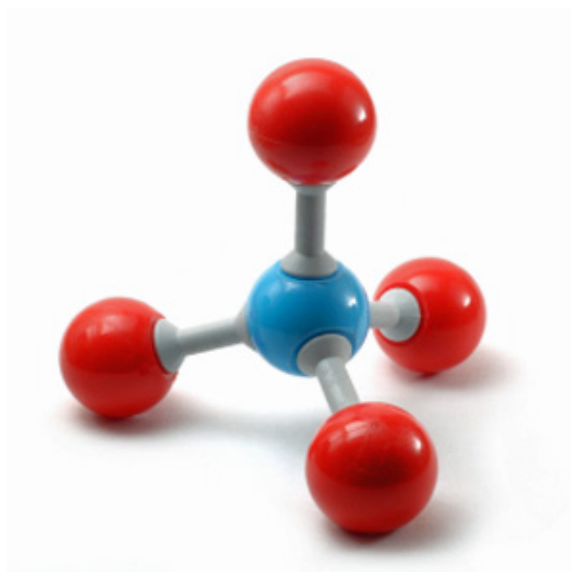
Our founding application is to measure the amount of excess ^{13}C-^{2}H “clumps” — two rare isotopes in the same molecule — in methane. This clumping, or nonrandom distribution, varies as a function of the temperature at which the molecule formed and equilibrated.

We are also working on methods to detect isotopic clumping in other molecules, as well as to detect the distribution of isotopes at specific positions within molecules.

Iso-what?

The “isotopic anatomy of molecules” may be a bit of a foreign concept. A bit of explanation …

Consider the molecule methane, comprised of 1 carbon atom bonded to 4 hydrogen atoms (shown at right). It has only one structure and always the same elements.



If you were handed a sample of methane and asked, “Where does it come from?” you might measure its concentration, but then what? At this level of detail, methane has essentially no distinguishing characteristics.

Fortunately, most elements come in different versions, called isotopes (https://en.wikipedia.org/wiki/Isotope).

Hydrogen has two stable isotopes (protium [^{1}H] and deuterium [^{2}H]), and carbon also has two (^{12}C and ^{13}C). So, in reality, there are actually 10 different isotopic versions of methane: $^{12}C^{1}H_4$, $^{13}C^{1}H_4$, $^{12}C^{1}H_3{}^{2}H$, $^{13}C^{1}H_3{}^{2}H$, etc. We call these different versions “isotopologs”, a contraction of ‘isotope’ and ‘homologs’. It turns out that some of the isotopologs are a tiny bit more stable than others. Specifically, the molecules with two or more rare isotopes (^{13}C or ^{2}H) bonded to each other (like $^{13}C^{1}H_3{}^{2}H$) gain extra stability from that interaction. As a result, they are marginally more abundant. The extent to which these molecules are more abundant (a property we call “clumpiness”) is a function of temperature; the cooler the temperature, the more “clumpy”.

Conventional stable isotope measurements (like $\delta^{2}H$ and $\delta^{13}C$) do not directly measure the individual isotopologs of methane. Instead, they convert them all to CO_2 and H_2, and then measure the total abundance of ^{2}H and ^{13}C. This provides some information about origins, but does not reveal the excess of $^{13}C^{1}H_3{}^{2}H$ that is needed to determine temperature. At Isotomics, we have developed advanced mass spectrometric capabilities that allow us to directly measure excess $^{13}C^{1}H_3{}^{2}H$ with a precision of better than 10 parts per million. From this measurement, we can predict the formation temperature of a methane sample to within 5°C.

For further, more technical details, please see the peer-reviewed journal articles below by Isotomics founders Eiler and Sessions.

- Eiler JM, Clog M, Magyar P, Piasecki A, Sessions AL, Stolper D, Deerberg M, Schlueter H-J, Schwieters J (2013) A high-resolution gas-source isotope ratio mass spectrometer. *International Journal of Mass Spectrometry*, **335**, 45-56.

- Stolper DA, Lawson M, Davis CL, Ferreira AA, Santos Neto EV, Ellis GS, Lewan MD, Martini AM, Tang Y, Schoell M, Sessions AL, Eiler JM (2014) Formation temperatures of thermogenic and biogenic methane. *Science* **344**, 1500-1503. DOI: 10.1126/science.1254509

- Stolper DA, Sessions AL, Ferreira AA, Santos Neto EV, Schimmelmann A, Shusta SS, Valentine DL, Eiler JM (2014) Combined ^{13}C-^{2}H and ^{2}H-^{2}H clumping in methane: methods and preliminary results. *Geochimica et Cosmochimica Acta* **126**, 169-191.

Why we do it

We are first bringing these tools to bear on problems in the energy industry, e.g. understanding the origins, migration and storage of natural gas and petroleum in the subsurface. Distinguishing biogenic from conventional thermogenic and “unconventional” (high-temperature) thermogenic gas is one concrete example. In the longer term, we are developing isotopic tools will become relevant to chemical synthesis and processing, pharmaceuticals, forensics, and perhaps biomedicine.

Who is involved

Isotomics was started by John Eiler and Alex Sessions, two professors of geochemistry at Caltech. Working in collaboration with ThermoFisher Scientific, they developed the analytical instruments, techniques, and methods that lead to the first “clumped-isotope thermometer” in methane. After many years of joint research projects with the energy industry, they founded Isotomics to commercialize these measurements. Other members of the Isotomics team include Nami Kitchen (Lab Manager), Mark Goodstein and Richard Weil.