

## High resolution mass spectrometry extends the limits of stable isotope geochemistry

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Conventional, low resolution isotope ratio mass spectrometry (IRMS) is established as the gold standard in stable isotope geochemistry. Applications include studies of atmospheric chemistry, (bio-)geochemical processes, and palaeoenvironmental reconstructions. Besides classical stable isotope methods, clumped isotope techniques, as well as position-specific isotope analysis have been progressively developed in recent years. However, measurements can be complicated by isobaric interferences from contaminants, adducts, and/or isotopologues.

High resolution isotope ratio mass spectrometry (HR-IRMS) overcomes these limitations by routinely achieving mass resolving powers of  $M/\Delta M > 30000$  (5, 95% edge definition). Here, we report the latest methods developed with the Thermo Scientific™ 253 Ultra™ high resolution gas source isotope ratio mass spectrometer:

(i) The first clumped isotope dataset for hydrogen [1] demonstrates the direct determination of  $\delta D$  and  $\Delta DD$  at natural abundance levels. (ii) A novel approach allows the direct determination of  $\delta^{13}C$  as well as triple oxygen isotope compositions from  $CO_2$  [2] with analytical precision of down to 15 ppm for  $\Delta^{17}O$ . (iii) Interference-free clumped isotope analyses of  $O_2$  [3] are performed at precision levels  $< 0.2$  ‰. (iv) Direct measurement of  $^{30}N_2$  [4] promises to improve on conventional denitrification measurement techniques [e.g. 5]. (v) Analyses of position-specific  $^{13}C$  distribution [6] and carbon clumping [7] in natural hydrocarbons provide novel tools to investigate petroleum systems.

HR-IRMS adds to the stable isotope geochemistry toolbox, by enabling direct (interference-free) measurements without the need for correction procedures, and by enabling novel applications that further explore the global atmospheric and petroleum systems.

[1] Popa *et al.* (2019) *RCMS* 33(3), 239-251. [2] Adnew *et al.* (2019) (under review). [3] Laskar *et al.* (2019) *RCMS*, doi: 10.1002/rcm.8434. [4] Albrecht (2019), Application Laboratory Thermo Fisher Scientific, Bremen (unpublished). [5] Well *et al.* (2018) *RCMS* 33(5), 437-448. [6] Piasecki *et al.* (2018) *GCA* 220, 110-124. [7] Clog *et al.* (2018) *GCA* 223, 229-244.