Initial results from the SUERC 253 Ultra: A new high resolution isotope ratio mass spectrometer for isotopologue analysis.

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A recent development in isotope ratio measurement has been the quantification of very small isotopic variations associated with doubly-substituted isotopologues. The integrity of ion beams at such low abundances is often compromised by isobaric contaminants and adducts with equivalent nominal mass. Resolving such interferences by increased mass resolution allows accurate quantification of low abundance ion beams.

The first of the next generation ThermoFisher Scientific 253 Ultra mass spectrometers will be delivered to SUERC in June 2015. The new instrument is a high resolution double-focusing IRMS. This instrument achieves mass resolving power of >>18,000 (M/ΔM, 5%, 95 % definition) and can analyze a wide range of diverse gases and semi-volatile compounds by dual inlet sample introduction.

The 253 Ultra has an advanced variable multi-collector array with 7 detector positions. 6 of the collectors can be moved automatically to allow simultaneous acquisition of the required masses in complex isotopologue systems. The collector array combines faraday detectors, electron multipliers and a high performance RPQ lens with the faradays having matrix switchable amplifiers (10^{10}, 10^{11}, 10^{12} gain), which can be deployed in variable relative mass configurations. A dynamic range of at least 10 orders of magnitude is thus available.

We report initial results from the new instrument which incorporates advanced design features that differ from the prototype CalTech 253 Ultra. New workflow oriented Qtegra software facilitates data evaluation and data acquisition for direct molecular isotope ratio analysis.

The 253 Ultra enables previously impossible isotopic analyses of gases and volatile organics and their fragment and adduct ions, such as: $\delta^{13}C$, δD and $^{13}CH_3D$ of methane; $\delta^{13}C$ of propane and many of its fragments (enabling position-specific ^{13}C determination); direct analysis of e.g. $\delta^{15}N$, $\delta^{17}O$, $\delta^{18}O$ and ^{15}N-^{18}O 'clumping' in N_2O and its fragments free of isobaric interferences.