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The new high-resolution IRMS MAT253 ULTRA at Utrecht University

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In 2016, the new high-resolution, multi-collector isotope ratio mass spectrometer MAT253 ULTRA [1] was installed at Utrecht University. This instrument is designed to reach a mass resolving power of 20,000 to 40,000 (M/ΔM). The ion currents are detected with a variable multi-collector unit that allows to register up to 9 ion currents simultaneously with Faraday cups and ion counters. The width of the entrance slit can be varied between 5 and 250μm so that the instrument can be operated under low, medium and high mass resolution, and an optimum balance between resolution and sensitivity can be selected for the respective applications.

The central field of application of the new IRMS at Utrecht University is the measurement of multiply substituted isotopologues (clumped isotopes) in atmospheric trace compounds (e.g. $^{13}CDH_3$, $^{13}C^{18}O^{16}O$, $^{18}O^{18}O$, $^{15}N^{14}N^{18}O$) [1-7]. It is known from thermodynamics that the zero point energy of a chemical bond usually decreases when multiple heavy isotopes clump together in a molecule, and this effect depends on temperature [7]. Therefore, the abundance of clumped isotopes can be used as temperature indicator under thermodynamical equilibrium conditions. However, in the atmosphere, many reactions are controlled kinetically. It has been shown recently for a few examples that negative clumping signatures (anti-clumping) can be produced under non-equilibrium conditions [3,4]. In addition, based on purely statistical reasons, anti-clumping signatures will be produced in any molecule that contains indistinguishable atoms, which originate from isotopically distinct reservoir [5,6]. Thus, the investigation of multiply substituted isotopologues is expected to generate novel isotope signatures that can complement conventional stable isotope analysis in atmospheric science. We will present data on the performance of the MAT 253 ULTRA instrument and first scientific applications to atmospheric research.

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