UNIT RESOLUTION MASS SPECTROMETRY OF THE ATMOSPEHRE OF VENUS.

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Analyses of unit-resolution mass spectra are complicated by numerous unresolved and overlapping peaks which are created by fragments of analyte molecules. The atmosphere of Venus is particularly susceptible to this problem, with overlapping peaks originating from CO2, N2, and CO (28 u); S- and O-bearing molecules (16, 32, 48 u); and P- and S-bearing molecules (32-36 u), among others. However, with precise calibration data and detailed instrument characterization, the effects of overlapping peaks can be mitigated, and the mass spectrum can be deconvolved into its component molecules.

To investigate this problem, we perform simulated retrievals of atmospheric composition by creating synthetic Venus mass spectrometer data and then deconvolving the spectra using the methods described by Gautier et al. (2020). We consider a wide variety of expected atmospheric compositions, as well as the effects of sample purification and enrichment, to determine whether important trace gases such as CH_4, NH_4, or PH_3 are detectable via mass spectrometry. We also assess the role of pre-flight calibration data in the spectral decomposition of our simulated in situ data.

Preliminary work shows that abundances for most gases can be retrieved with ~10% precision, provided the gas' base peak is free from contamination. For example, SO_2, with a base peak of 64 u, is easily retrieved with accuracy < 5% and precision < 10%, despite many overlapping fragment peaks at 48 u, 32 u, and 16 u. However, CO, with a base peak of 28 u (overlapping with N_2) is not possible to measure accurately with unit-resolution mass spectrometry. Isotope ratios for carbon, oxygen, and sulfur can be retrieved at sub-percent levels with precise pre-flight calibration, i.e., if molecular fragmentation patterns are known to within 2%. Due to numerous peak overlaps, the precision of the retrieved D/H ratio is limited to about 15%.

Future work will explore the synergies between mass spectrometry and simultaneous infrared spectroscopic measurements of atmospheric gases and isotope ratios to improve constraints on atmospheric composition.