DETECTING AND IDENTIFYING VOLATILE ORGANIC SUBSTANCES USING INFRARED SPECTROSCOPY COMBINED WITH PHASE DIAGRAMS.

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Introduction: Detecting trace-level organic matter in rock and dust is specified as a challenge area in the project synopsis. Volatile organic substances (VOS) can be released from rock or dust by heating the samples to elevated temperatures. Our proposal is to use a combination of fingerprint infrared spectroscopy and simultaneous temperature and pressure detection for obtaining phase diagrams. With this combination of techniques, it is not only possible to detect the existence of trace-level VOS, but also to identify the nature and structure of these substances. These tools are lightweight, easy to implement, cost effective and enable gathering and analyzing of vital data on a continuous basis.

Why VOS? Volatile organic substances, such as methane and other hydrocarbons, terpenes, ethers, even water,… are connected to the existence of biomass or an indication of life once existing on the planet. Trace-level detection of these compounds thus allows for the direct or indirect discovery of life, water or biomass deposits (such as oil) on Mars.

Evaporation of susbstances from samples: Interesting samples should be brought into a heating oven. The elevated temperature in the oven will then release the volatile molecules present in the sample and make them available for gas-phase detection.

Fingerprint infrared spectroscopy: Infrared spectroscopy (IR) is a very suitable technique for the detection of organic and water molecules in the gas phase. Readily detectable molecules include water, CO_2, hydrocarbons, ethers,… Analysis of spectral infrared data allows for identification of present chemical compounds, groups and elucidation of chemical structure. [1] Infrared spectroscopy is already a heavily used tool in astronomical research for investigation of e.g. atmospherical compositions. [2]

Simultaneous temperature and pressure detection: Using a temperature and a pressure sensor in the oven and simultaneously monitor both parameters it is possible to construct phase diagrams of the detected substances. From these phase diagrams, information can be inferred concerning phase transitions, compositions of mixtures, vapor pressures, quantities of detected molecules and more.

Combination of infrared spectroscopy and phase diagrams: This combination of techniques leads to a powerful analytical toolbox for the detection and identification of molecules present in interesting Martian rock or dust samples. As molecules evaporate from the samples due to heat from the oven, the pressure in the oven at that certain temperature will change over time indicating the presence and vapor pressure of the compound. Together with this information, the infrared spectrum of the present molecule(s) is recorded. After combining the acquired information, one can obtain a data set of time-resolved pressures and infrared spectra per degree of oven temperature. This data

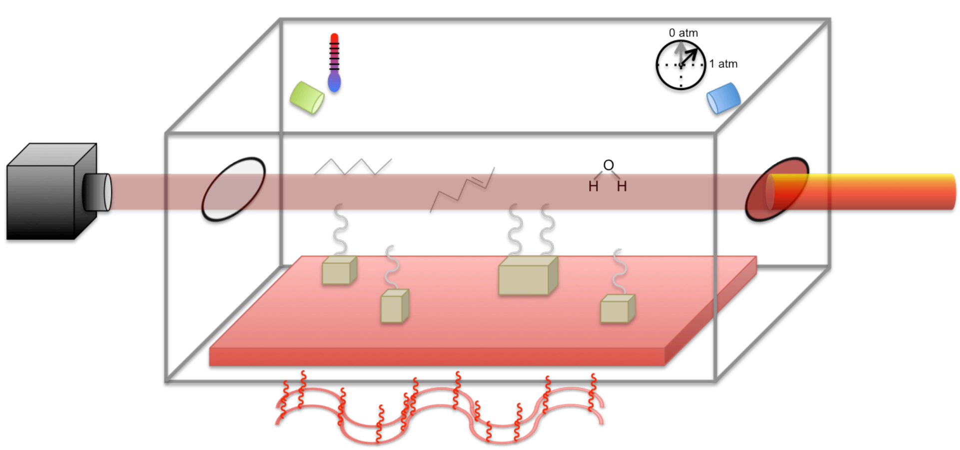

Figure 1: Visual representation of the envisioned setup.

set allows the identification of molecules present at that certain temperature and thus in the Martian sample. As such, the combination of two straightforward, easy to implement, light-weight and cost-effective techniques allows for very advanced analysis of Martian samples.

Practical setup: A representation of an envisioned setup is shown in Figure 1. Central in the image is the oven, heated by a resistor underneath. As samples are heated, volatile molecules are released from the sample. While the oven is heated, the temperature and pressure in the oven are monitored by sensors. Infrared light enters the oven through an optical window on the right side. The source of the infrared light can be the sun, radiation from stars or an infrared light source. The light beam then passes through the oven filled with molecules in the gas phase, acquiring information about those molecules. An optical window on the left side of the window allows clean transmission of the light beam to the detector. To obtain a spectrum, separation of wavelengths is necessary. There are multiple possibilities to achieve this separation, e.g. a prism or a grating after the light beam has exited the oven or selecting wavelengths before it is transmitted through the oven by a grating, cut-off or bandpass filters or a full featured monochromator.

An interesting intermediate advanced solution for wavelength selection is using a changeable filter wheel before the oven. With such a filter wheel one could select a certain number of infrared wavelengths for detection. Interesting wavelengths in the infrared are those for the characteristic groups such as amines, alcohols or cyanides and molecules such as CO_2 and H_2O. The combination with simultaneous temperature and pressure detection ensures proper detection and identification of compounds.

Required components: Minimal required components are a cut-off or bandpass filter for incoming wavelength selection, a heating element, temperature and pressure sensors and a detector, which can be a CCD camera, a photomultiplier tube or even photodiodes, depending on the desired resolution and acquiring time. This minimal setup would be very light-weight, cost-effective and easy to implement.

This minimal setup could be complemented by the filter wheel wavelength selection as explained in the previous section as an intermediate solution.

A more extensive setup would include a monochromator for incoming light wavelength selection and a spectral detection method such as an array of photodiodes. This setup would be somewhat more expensive and more difficult to implement but would yield more complete datasets for analysis.

Conclusion: By using a combination of fingerprint infrared spectroscopy and simultaneous temperature and pressure monitoring, advanced detection, identification and quantification of VOS in rock and dust material becomes feasible. The required components are-light-weight, cost-effective and easy to implement which is are major advantages for planetary exploration missions.

References:

[1] Banwell C. N. and McCash E. M. (1994) *Fundamentals of Molecular Spectroscopy,* 4^{th} ed. McGraw-Hill Companies.

[2] Hanel R. A. et al. (2003) *Exploration of the solar system by infrared remote sensing,* 2^{nd} ed. Cambridge University Press.