SAM GCMS Calibrations for Identification of Organics on Mars

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Introduction:

Goal:

To calibrate the relative retention times of expected Mars analyte components to SAM internal standards.

Abstract:

Sample Analysis at Mars (SAM) is located on the Curiosity Rover that will land on Mars on August 5, 2012. SAM contains a Gas Chromatograph Mass Spectrometer (GCMS), which will be used by scientists to identify organic molecules if present on Mars. Organic molecules will be identified based on mass spectra and GC retention time (i.e., amount of time it takes for a molecules to pass through the GC column). SAM will use its internal standards as markers for retention times. We analyzed mixtures of organic molecules and calibrated the retention times of the analyte components to SAM internal standards. The relative retention time between the sample mixture components and the internal standards act as identification markers. These relative retention time markers will be used during SAM operations to help identify if and what organics are present on Mars.

Materials &Methods:

Pyrolyzer:

A sample is placed in a stainless steel cup in the Pyrolyzer. In the Pyrolyzer, the cup drops into a heated zone. The temperature is then ramped to 1000° C. Gas evolved from the heated sample exit the Pyrolyzer and enter the cool (10° C) Gas Chromatograph (GC)

Gas Chromatograph Mass Spectrometer (GCMS):

Gas Chromatograph

The molecules of the evolved gas move through the GC column at speeds based on the properties of the molecules, molecular interactions with the column film, and the temperature of the oven. The oven is ramped from 10° C to 300° C at different rates (3, 6, & 10 C/min), similar to the range SAM might use on Mars. As the molecules move through the column, they become separated and reach the Mass Spectrometer (MS) at different times

• SAM contains 4 columns designed for different types of molecules. The RTX-5 Column used here is appropriate for non-polar to slightly polar hydrocarbons.

Mass Spectrometer

The MS produces electrons and directs them towards the incoming molecules. The molecules are then ionized and directed towards a detector. The data from the sample collected consists of a chromatogram showing peak relative abundance and retention time as well as associated mass spectra for each peak.

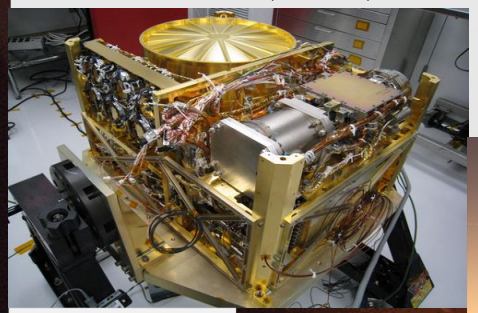

Figure 1.
Sample Analysis at Mars (SAM). SAM consists of a GCMS that allows for identification of organics potentially discovered on Mars.

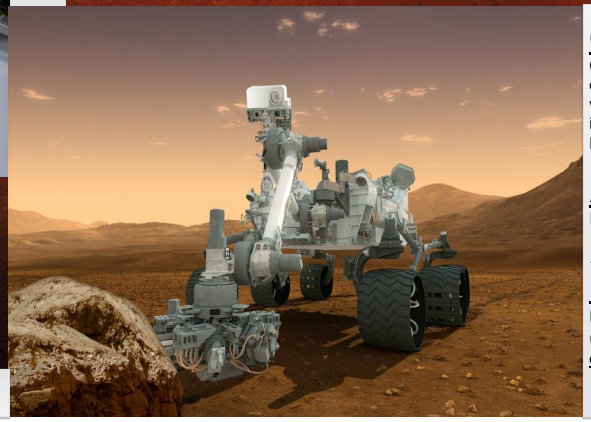

Figure 7.
Curiosity Rover that contains SAM

Data:

The relative retention times in the charts displayed below, are ratios of where on the chromatogram a specific organic will be. No two columns are the same, therefore for example, Phenanthrene will not come off the column at an absolute time, every time when two different columns are used. Thus, calculating relative retention times to internal standards allows the identification of organics by retention time to be standardized to any column used.

Alkanes

Alkane	GC 3C/min Ramping Retention Time 1-FN	GC 3C/min Ramping Retention Time PFBP	GC 6C/min Ramping Retention Time 1-FN	GC 6C/min Ramping Retention Time PFBP	GC 10C/min Ramping Retention time 1-FN	GC 10C/min Ramping Retention Time PFBP
Decane	0.56	0.51	0.61	0.57	0.64	0.61
Undecane	0.76	0.70	0.79	0.74	0.79	0.76
Dodecane	0.93	0.86	0.94	0.88	0.93	0.90
1-Tetradecene	1.21	1.12	1.19	1.11	1.14	1.10
Pentadecane	1.34	1.24	1.30	1.22	1.24	1.19
Hexadecane	1.47	1.36	1.40	1.31	1.34	1.28
Heptadecane	1.58	1.46	1.50	1.41	1.42	1.37
2,6,10,14-Tetramethyl Pentadecane	1.61	1.48	1.53	1.43	1.44	1.38
Octadecane	1.69	1.57	1.60	1.49	1.51	1.45
Eicosane	1.90	1.76	1.77	1.66	1.66	1.59
Henecosane	2.09	1.93	1.93	1.81	1.80	1.73
Tetracosane	2.26	2.09	2.08	1.95	1.93	1.85
Hexacosane	2.42	2.24	2.22	2.08	2.05	1.97
Octacosane	2.57	2.38	2.34	2.19	2.16	2.07
Triacontane	2.71	2.50	2.46	2.30	2.26	2.17

Figure 2.
The data table consists of the relative retention times of the Alkanes to the SAM internal standards. The data table depicts how far away each alkane elutes from each SAM standard on the chromatogram.

PAHs

PAH	GC 10C/min Ramp Retention Time 1-FN	GC 10C/min Ramp Retention Time PFBP
Naphthalene	1.11	1.07
Acenaphtheylene	1.28	1.23
Acenaphthene	1.29	1.24
Fluorene	1.40	1.34
Phenanthrene	1.42	1.36
Anthracene	1.58	1.52
Fluoranthene	1.59	1.53
Pyrene	1.81	1.74
Benzo(a)Anthracene	1.85	1.77
Chrysene	2.07	1.98
Benzo(b) Fluoranthene	2.08	1.99
Benzo(k) Fluoranthene	2.26	2.17
Benzo(a)Pyrene	2.27	2.18
Indeno(1,2,3-cd)Pyrene	2.31	2.22
Benzo(a,h,)Anthracene	2.50	2.40
Benzo(g,h,I,)Perylene	2.54	2.44

Figure 3.
The data table consists of the relative retention time of the16-PAHs to the SAM internal standards. The data table depicts how far away each PAH elutes from each SAM standard on the chromatogram

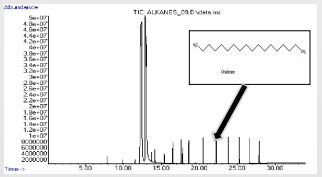

Figure 4a.
The chromatogram consists of Alkanes and the SAM standards (1-FN and PFBP). The chromatogram depicts when each alkane elutes from the column relative to when the SAM standards elute.

Figure 4b.
Octadecane. One of the alkanes present in the chromatogram.

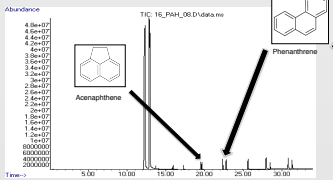

Figure 5a.
The chromatogram consists of 16 PAHs and the SAM standards (1-FN and PFBP). The chromatogram depicts when each PAH elutes from the column relative to when the SAM standards elute.

Figure 5b.
Acenaphthene. One of the PAHs present in the chromatogram.

Figure 5c.
Phenanthrene. One of the PAHs present in the chromatogram.

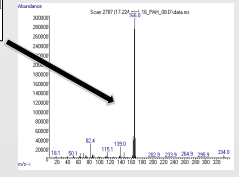

Figure 6.
The mass spectra consists of the different molecular fragments that make up the PAH Phenanthrene. The mass spectra allows for the identification of a compound that is represented as a peak in the chromatogram.

Conclusion:

Calculating the relative retention times of known, common organic molecules to the SAM internal standards will be used to verify the presence or absence of certain molecules and will help in the identification of other organic molecules encountered on Mars.

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Further Information:

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