Space Science Division

1998 Annual Report

NASA Ames Research Center
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COVER ART: Artist's concept of the brilliance and beauty of a sun at the center of some solar system; a welcoming beacon in the darkness of space. (Artwork: James Schilling)

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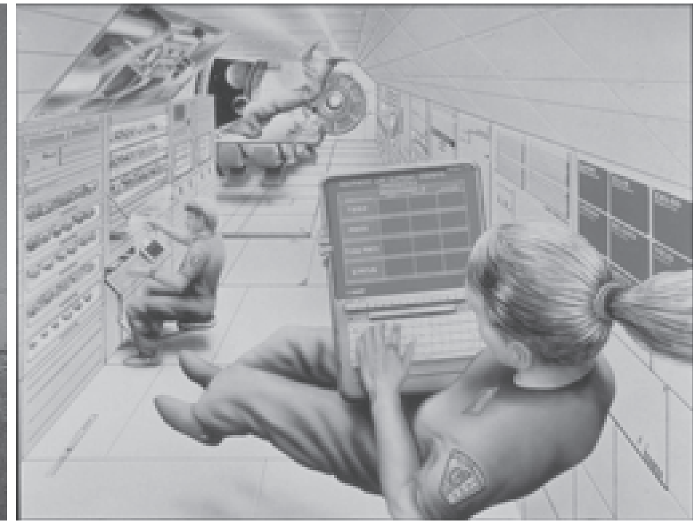
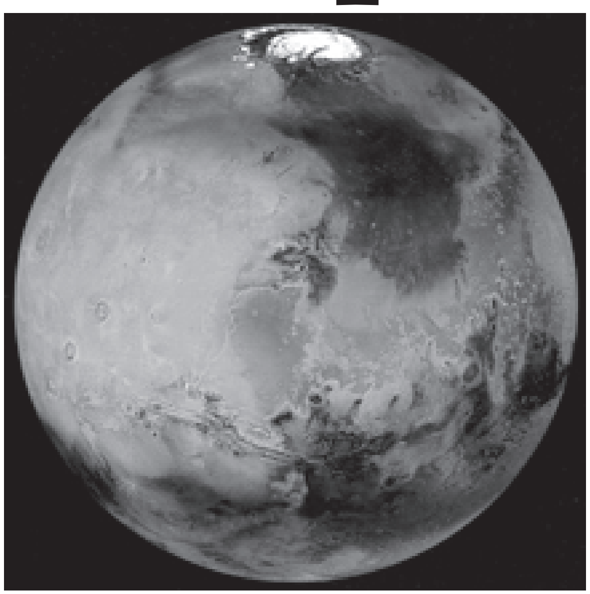
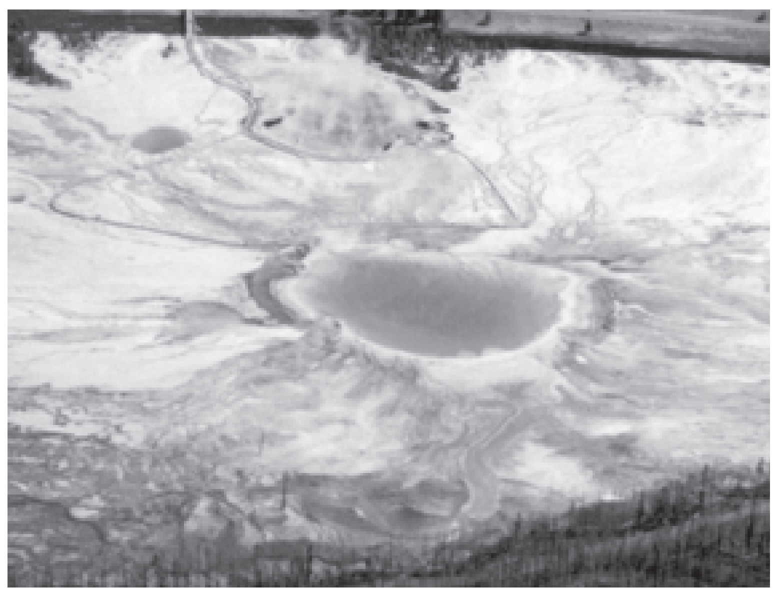


Space Science Division





Annual Report

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DIVISION OVERVIEW

The Space Science Division at NASA's Ames Research Center conducts research programs that are structured around the study of the origins and evolution of stars, planetary systems, and life, and that address some of the most fundamental questions pursued by science, questions that examine the origin of life and of our place in the universe, and questions that lie at the heart of the emerging discipline of Astrobiology.

Ames is recognized as a world leader in Astrobiology, defined as the study of life in the universe and the chemical and physical forces and adaptations that influence life's origin, evolution, and destiny. In pursuing this primary Center mission in Astrobiology, scientists in the Space Science Division perform pioneering basic research and technology development to further fundamental knowledge about the origin, evolution, and distribution of life within the context of cosmic processes. To accomplish this objective the Division has assembled a multidisciplinary team of scientists including astronomers, astrophysicists, chemists, microbiologists, physicists, and planetary scientists. It also requires access to the space environment, since many of the critical data needed to elucidate the evolutionary steps outlined above are only available in space in star-forming regions, in the interstellar medium, and in and around planetary environments.

Major elements of the Space Science Division's program include the study of the interstellar gas and dust that form the raw material for stars, planets, and life; the processes of star and planet formation; the evolution of planets and their atmospheres; the origin of life and its early evolution on the Earth; the search for past or present life throughout the solar system with emphasis on Mars; and life support systems for human solar system exploration missions.

Space Science Division personnel participate in a variety of major NASA missions. Division scientists are/were Investigators, Team Members, or Interdisciplinary Scientists on Pioneer, Voyager, Galileo, the Ulysses space physics mission, the Japanese cooled space infrared telescope (IRTS), the Cassini mission to Saturn, and the Kuiper Airborne Observatory. Division scientists are involved in the development of the Stratospheric Observatory for Infrared Astronomy (SOFIA), planetary detection with Kepler, Stardust, the Mars Surveyor program, the Space Infrared Telescope Facility (SIRTF), and Next Generation Space Telescope (NGST).

The programs in the Space Science Division are international in scope, ranging from active participation in international scientific meetings and societies, to collaborative ground-based research projects, to scientific investigations on international flight missions and projects.

Extensive ties are maintained with the academic community through collaborative research programs and development of science curricula materials, and additionally, students at all levels represent a significant component of the Division's on-site research work force.

The Space Science Division represents a unique resource for NASA's Astrobiology Initiative and in support of the Agency's current and future manned and unmanned missions. The science and mission capability of the Space Science Division described here is unmatched by any other NASA Center or national laboratory.

The Division is organizationally divided into four Branches (see Figure 1) named according to the focus areas of the research conducted by the scientists in those Branches: Astrophysics, Astrobiology Technology, Exobiology, and Planetary Systems.

In 1998, the Division employed 70 Civil Service personnel, 45 of whom are Ph.D. scientists. This core permanent staff is augmented with approximately 150 scientists and technicians who are non-civil servants resident in Division facilities through mechanisms such as grants, cooperative agreements, support contracts, fellowships, visiting scientist positions, and student internships.

It is common for visiting scientists from U.S. universities to spend their summer research or sabbatical time in the Division's laboratories and facilities. Extensive ties are maintained with the academic community through collaborative research programs and also through the development of science curricula materials. The Space Science Division is dedicated to fostering greater interest in careers in the sciences and provides unique opportunities for training the next generation of scientists. Students at all levels – high school, undergraduate, graduate, and post-doctoral – represent a significant component of the Division's on-site research work force. In 1998, 21 National Research Council Postdoctoral Fellows were resident in the Division, 8 undergraduate students were employed through various internship programs, and Division personnel managed the Astrobiology Academy, a competitive program for college undergraduates to participate in hands-on research projects here at Ames Research Center.

In the following section of the Annual Report, the research programs of each Branch are summarized. Within each area, several examples of research topics have been selected for more detailed description. Following that section is a list of publications authored by Division personnel with 1998 publication dates. Finally, if a particular project is of interest, the personnel roster that begins on page 81 may be used to contact individual scientists. ❑

Donald L. DeVincenzi
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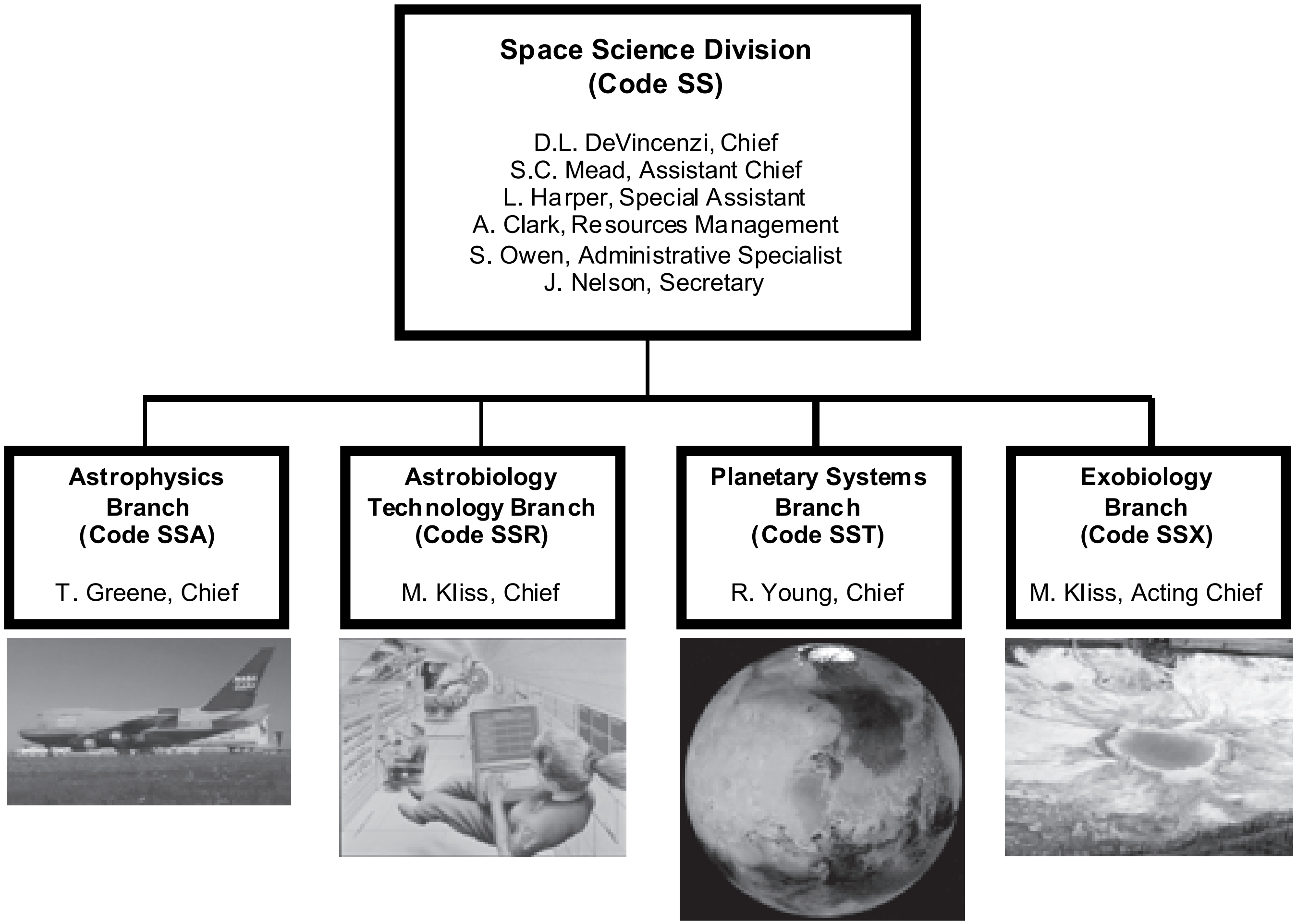
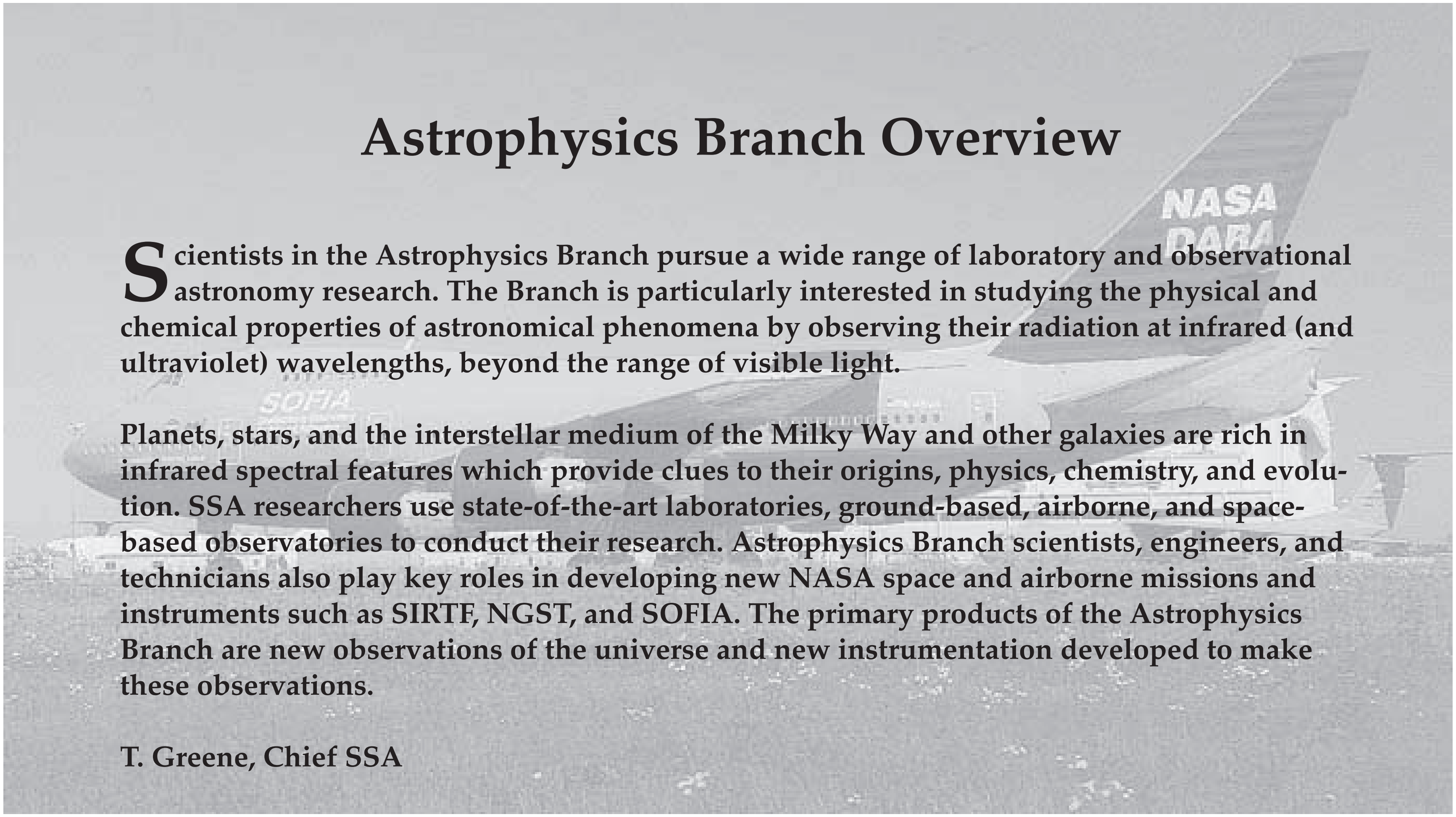


Figure 1. Space Science Division organization chart.



Astrophysics Branch Overview

Scientists in the Astrophysics Branch pursue a wide range of laboratory and observational astronomy research. The Branch is particularly interested in studying the physical and chemical properties of astronomical phenomena by observing their radiation at infrared (and ultraviolet) wavelengths, beyond the range of visible light.

Planets, stars, and the interstellar medium of the Milky Way and other galaxies are rich in infrared spectral features which provide clues to their origins, physics, chemistry, and evolution. SSA researchers use state-of-the-art laboratories, ground-based, airborne, and space-based observatories to conduct their research. Astrophysics Branch scientists, engineers, and technicians also play key roles in developing new NASA space and airborne missions and instruments such as SIRTF, NGST, and SOFIA. The primary products of the Astrophysics Branch are new observations of the universe and new instrumentation developed to make these observations.

T. Greene, Chief SSA

Ices in Kuiper Disk Objects

Dale P. Cruikshank, Yvonne J. Pendleton, Robert H. Brown and Glenn J. Veeder

Beyond the planet Neptune lies a disk-shaped distribution of small, primitive bodies called the Kuiper Disk. This region is named after the prominent astronomer, Gerard P. Kuiper, who predicted its existence in 1951. Kuiper speculated that such a population of objects must exist in order to explain the orbital characteristics of the short-period comets (periods less than 200 years) that currently come to the inner part of the Solar System at the rate of about 10-20 per year. The first of these 'trans-Neptunian' objects was found in 1992, and about 80 of them have been detected as of January 1999. Their dimensions are approximately 50 to 500 kilometers; much smaller ones surely exist but are too faint to be found with telescopes presently available. Because these bodies are implicated in the transport of volatiles and complex organic materials to the pre-biotic Earth and other terrestrial planets, Ames scientists have conducted astronomical observations to establish their compositions.

The trans-Neptunian objects are expected to be composed of the same materials that make up the short-period comets, which are typically one-third ices of frozen water, carbon dioxide, carbon monoxide, and others, one-third silicate dust, and one-third complex organic solid material. Remote sensing measurements of these bodies to establish their compositions and to search for variations among them are a challenge for presently available astronomical techniques; only the largest 15-20 bodies can be observed with infrared spectrometers on the world's largest telescopes.

A new Ames spectroscopic study with the Keck 10-meter telescope on Mauna Kea, Hawaii, is showing that the trans-Neptunian objects are diverse in their surface compositions. At least one (designated 1993 SC) shows evidence for hydrocarbon ices (possibly methane), while others show the spectroscopic signature of frozen water. In addition, the strong red color of the surfaces of several of these bodies is evidence for the presence of organic solid material that has been produced in interstellar space and further processed since incorporation into the Solar System. The color and spectral properties of the red trans-Neptunian objects are closely matched by "tholins," which are complex organic materials synthesized in the laboratory by the irradiation of simple gases and ices with ultraviolet light and charged particles.

The results of the spectroscopy of ten trans-Neptunian objects, their 'cousins' the Centaurs (bodies in temporary orbits that cross the paths of the major planets), and the irregular outer satellites of the major planets shows that they are compositionally diverse. The planet Pluto and Neptune's satellite Triton probably represent two of the largest bodies in the Kuiper disk population, and each of these two bodies has a complex icy surface and a tenuous atmosphere. The Ames study includes remote sensing observations of all these objects, in search for unifying threads of evidence that may link their compositions with the comets and other bodies that have impacted Earth and the other planets, bringing volatile and organic matter from the most distant reaches of the Solar System. ❑

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AIRES - A Facility Spectrometer for SOFIA

Edwin Erickson, Michael Haas, and Sean Colgan

The Stratospheric Observatory for Infrared Astronomy (SOFIA) is an airborne telescope facility currently under development and construction. A Boeing 747 will be equipped to carry a 2.7-meter telescope to be operated altitudes up to 45,000 feet. Thus, SOFIA will enable astronomical observations with unprecedented angular resolution at infrared wavelengths that are obscured from the ground. It is being developed jointly by NASA and DLR, the German Aerospace Center. It will be based at Ames Research Center and will begin operations in 2002.

An Ames team led by Ed Erickson, Mike Haas, and Sean Colgan were one of six American groups selected by peer review to build a focal plane instrument for early observations with SOFIA. The Ames instrument, AIRES, the Airborne Infrared Echelle Spectrometer, will be a general-purpose facility instrument. After development by the Ames team, it will be operated for the science community by the Universities' Space Research Association (USRA), NASA's prime contractor for SOFIA.

AIRES will operate at far infrared wavelengths, roughly 30 to 400 times the wavelengths of visible light. This means it will be ideal for spectral imaging of gas-phase phenomena in the interstellar medium (ISM), the vast and varied volume of space between the stars. Measurements of far infrared spectral lines with AIRES will probe the pressure, density, luminosity, excitation, mass distribution, chemical composition, heating and cooling rates, and kinematics in the various gaseous components of the ISM. These lines offer invaluable and often unique diagnostics of conditions in such diverse places as star forming regions, circumstellar shells, the Galactic Center, starbursts in galaxies, and the nuclei of active galaxies energized by accretion of material on massive black holes. AIRES will provide astronomers with new insights into these and other environments in the ISM. It will also be useful for studies of solar system phenomena such as planetary atmospheres and comets, and a variety of other astronomical problems.

The AIRES design incorporates what will be the world's largest monolithic (echelle) grating (see Figure 2), and four different types of infrared array detectors operating at temperatures between 2 and 8 degrees Kelvin. In the past year the team has demonstrated that this cryogenic optical system can be designed to achieve the theoretically limited performance required by AIRES. Development of a comprehensive data system and associated software system, which will permit effective utilization of AIRES, is well underway. ❏

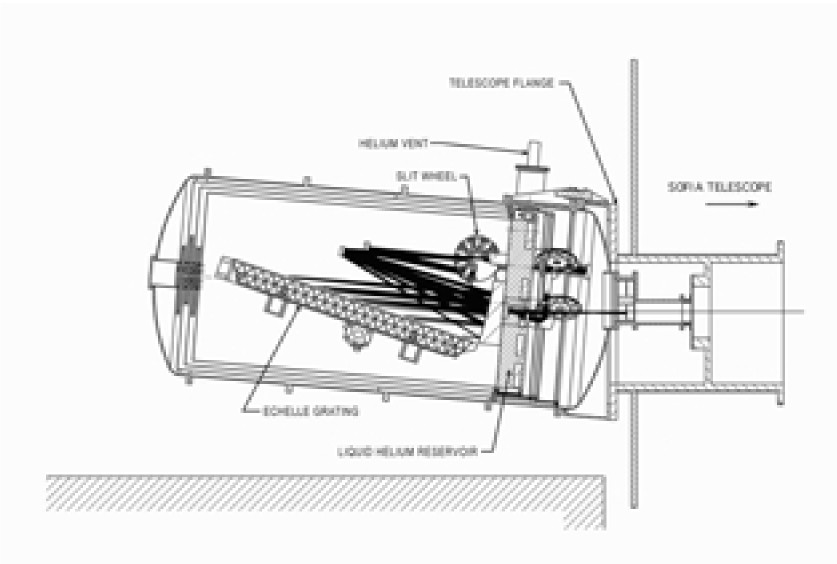

Figure 2. The AIRES design concept is shown; the echelle grating is roughly 42 inches long.

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Calculation of Instrument Functions

David Goorvitch

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In many situations, analysis of a spectrum is contingent on knowing the response of the measuring instrument. One popular analytical method is to obtain these instrumental parameters by iteratively fitting a theoretical spectrum to the observed spectrum until they match. This method involves convolving the theoretical spectrum with the response function of the measuring instrument. The iteration process is usually a nonlinear process and is repeated many times to reach convergence of the theoretical and observed spectra. Since the instrument response function is convolved with the theoretical spectrum in each measurement, accurately knowing the response function can eliminate potential errors in the derived spectroscopic information. A new Ames study has shown how instrument response functions can be calculated more rapidly and accurately.

The calculation of a response function, more commonly called the instrument function, is complicated even in a simple case. The complication arises when the instrument function is made up of several effects. For example, the mathematical instrument function for the Fourier transform spectrometer, even for the unapodized case, is composed of a rectangle representing the physical travel of the instrument and a 'sinc' function (equal to the sin function divided by its argument) representing the collimation of the beam. Each of these functions is also well described in the frequency realm of the measured spectra. However, the composite mathematical instrument function results in an integral of a sinc function between finite limits. This integral can not be represented as a simple analytical function, so it must be approximated.

A new Ames research effort has attacked this problem by transforming it into the orthogonal physical space where its equations can be solved analytically or by a simpler approximation. Transformation to an orthogonal space is facilitated by the convolution theorem, which states that the convolution of two functions can be obtained by multiplying their transforms and then back transforming to the original space. In addition, the convolution theorem has the added advantage that calculating the Fourier transform and inverse Fourier transform is faster than computing the direct calculation of the convolution. The computing time it takes to perform a transformation using the fast Fourier transform is proportional to $N \log_2 N$, while the direct convolution time is proportional to N_2. Thus this new technique has a potential savings in computational time of which is proportional to $N/\log_2(N)$ for N measurements in each spectrum.

This study has shown the power of using the convolution theorem in calculating instrument functions in several examples including an apodized Fourier transform spectrometer which is illuminated with uncollimated radiation and whose mirrors are misaligned. The instrument functions in these cases are far from ideal, but the new technique was successful in calculating them quickly and accurately. ❏

Organic Molecules in Comets

B.N. Khare, S.J. Clemett, R.N. Zare, and D.P. Cruikshank

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Comets are the oldest, most primitive organic-rich bodies in the Solar System, and they have preserved in them the earliest record of material from the nebula in which the Sun and the planets formed.

Simulations of the organic molecules in comets are undertaken in the Cosmochemistry Laboratory at Ames. Mixtures of ices comprised of various combinations of simple molecules are irradiated with sources of energy such as ultraviolet light and charged particles. This results in the formation of colored solids of low volatility which, when analyzed reveal a complex array of polymers, C_1 through C_5 hydrocarbons, nitriles, alkanes, alkenes, and nitrogen heterocyclic compounds. This colored solid material is collectively termed 'tholin.' The complex optical indices of this solid material are determined over a wide range of wavelengths, so that those indices can be used in mathematical models of the spectra of comets, planetary satellites, and other bodies of the Solar System. Tholins formed by irradiating various initial combinations of ices (and gases) appear to be uniquely capable of providing the coloration and spectral properties observed telescopically in many Solar System bodies.

In a particular experiment designed to simulate the solid organic material in comets, Ice Tholin I was produced by the irradiation of a mixture of H_2O (water) and C_2H_6 (ethane) ices present in a 6:1 ratio. Analysis of the solid residue produced by the irradiation was accomplished with the newly developed technique of microprobe two-step laser mass spectrometry (L^2MS) in the laboratory of R. Zare (Stanford University). The analysis revealed for the first time the presence of polycyclic aromatic hydrocarbons (PAHs) in tholins. A PAH-containing Ice Tholin II (see figure 3) was produced from a more complex mixture of ices made of H_2O, CH_3OH (methanol), CO_2 (carbon dioxide), and C_2H_6 (ethane) in the ratio 100:20:4:1. This mixture of four ices closely simulates the composition of comets.

In Ice Tholin I the PAHs are not distributed uniformly, but are found in microscopic concentrated regions where the concentration is greater than 300,000 parts per million. The PAH distribution in Ice Tholin I is characterized by simple 1-, 2-, and 3-ring PAH species with extensive side-chain alkylation (replacement of -H with $-(CH_2)_nH$). In Ice Tholin II, the PAHs are distributed more uniformly; naphthalene and its n=1 and n=2 alkylated homologues dominate.

The detection of PAHs in laboratory simulations of comets opens the pathway to the interpretation of PAHs found in the comet particles that are collected in the Earth's high stratosphere (interplanetary dust particles), and those collected at Comet P/Wild 2 and returned to Earth by the Stardust mission early in the next Century. ❏

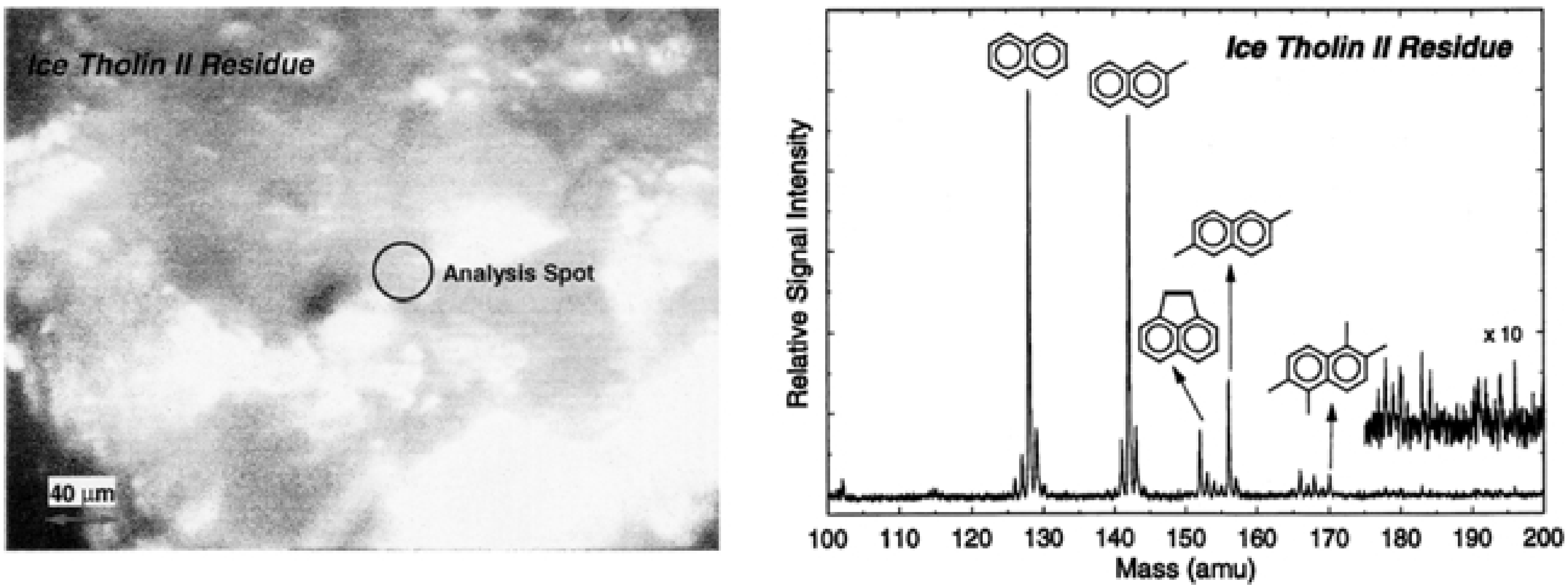

Figure 3. Photomicrograph of a film of Ice Tholin II, showing the area in which the two-step laser technique detected polycyclic aromatic hydrocarbons.

A Testbed for Detection of Earth-Sized Planets

David Koch, William Borucki, and Larry Webster

Detection of Earth-size planets beyond our solar system is one of the fundamental goals identified in NASA's Strategic Plan. Only in recent years have planets of any size been detected beyond our solar system. Those found to date are all on the order of the mass of Jupiter or larger. The challenge is to find planets which are 30-600 times less massive than Jupiter, i.e., one-half to ten times the mass of the Earth. The concept for a space-based instrument to accomplish this goal has been developed and named the *Kepler Mission*.

If most stars like the Sun have planetary systems similar to our own, it is estimated that this mission would discover on the order of 500 habitable planets. The capabilities have been set high, so that if no such planets are detected this 'null result' would have a profound impact on our understanding of planet formation. The mission concept is to continuously and simultaneously monitor the brightness of 100,000 solar-like stars. The 'light-curves' for each star are analyzed for fluctuations due to transits of Earth-size planets. Light-curves measured during three transits across a star, all with consistent period, brightness change, and duration, will provide a rigorous method of detection and confirmation. The size of a planet can be calculated from the relative brightness change that occurs during transit, and the orbital size can be calculated and the planet's temperature estimated from the period.

At the heart of the proposed Kepler Mission is an instrument containing an array of charged-coupled-device (CCD) detectors for measuring stellar brightness. These devices are similar in principle to those used in video cameras but are much larger in size and more sensitive. The critical property of the CCDs is their relative photometric precision, that is, how well they can measure the brightness of a given star relative the average brightness of the many thousands of stars nearby.

To demonstrate this, a testbed is being constructed which will utilize a CCD similar to that being proposed for the space-based mission, however, the test will view a star field with a ground-based instrument. The objective of the current testbed project is to demonstrate the technological readiness of the mission. Unfortunately, distortions caused by the atmosphere prevent measuring to the relative precision required which is 1 part in 100,000; the best photometric precision that has been achieved from the ground is only somewhat better than 1 part in 1,000. This is why the planet-detection goal cannot be achieved with a ground-based instrument looking through the atmosphere. To overcome this problem in the test and demonstrate that the CCDs do have the inherent relative precision required, an instrument is being constructed in which a calcite beam splitter is placed in front of the CCD. This produces a pair of identical images on the CCD. The photometric capability of the CCDs will be demonstrated by comparing the ratios of the brightness for each star pair. The instrument for performing these measurements is currently being constructed. Successful completion of the test should demonstrate the technology readiness for a space mission.

For further information on the proposed *Kepler Mission*, see the world wide web at: http://www.kepler.arc.nasa.gov ❑

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The SOFIA Water Vapor Monitor

Thomas L. Roellig, Robert Cooper, Anna Glukhaya, and Michael Rennick

As part of the development of the Stratospheric Observatory for Infrared Astronomy (SOFIA), scientists at Ames Research Center have developed an instrument that will measure the amount of water vapor seen along the telescope line-of-sight. Since the presence of water vapor strongly affects the astronomical infrared signals detected, such a water vapor monitor is critical for proper calibration of the observed emission. The design of such a water vapor monitor is now complete.

The SOFIA water vapor monitor measures the water vapor content of the atmosphere integrated along the line of sight at a 40° elevation angle by making radiometric measurements of the center and wings of the 183.3 GHz rotational line of water. A picture of this water vapor line as it would appear from SOFIA, together with the measurement bands of the SOFIA water vapor monitor, is shown in Figure 4.

The SOFIA water vapor monitor must provide knowledge of the amount of precipitable water vapor to 2 microns or better, 3-sigma, measured at least once a minute, along the telescope line-of-sight. In addition, knowledge of the water vapor to the zenith is needed to equivalent accuracy. Water vapor levels along other telescope lines-of-sight or to the zenith will then be determined by calculation from the 40° measurements. This imposes more restrictive accuracy requirements on the water vapor monitor sensitivity, namely 1.33 microns precipitable, 3-sigma, measured at least once a minute. The monitor hardware consists of three physically distinct sub-systems:

1) The Radiometer Head Assembly, which contains an antenna that views the sky, a calibrated reference target, a radio-frequency (RF) switch, a mixer, a local oscillator, and an intermediate-frequency (IF) amplifier. All of these components are mounted together and are attached to the inner surface of the aircraft fuselage, so that the antenna can observe the sky through a microwave-transparent window.

2) The IF Converter Box Assembly, which consist of IF filters, IF power splitters, RF amplifiers, RF power meters, analog amplifiers, A/D converters, and a RS-422 serial interface driver. These electronics are mounted in a cabinet just under the radiometer head and are connected to both the radiometer head and the water vapor monitor computer.

3) A host computer that converts the radiometer measurements to measured microns of precipitable water and communicates with the rest of the SOFIA mission and communications control system. These electronics are located in a rack elsewhere in the aircraft and are connected to the drive electronics through a RS-422 serial line. ❑

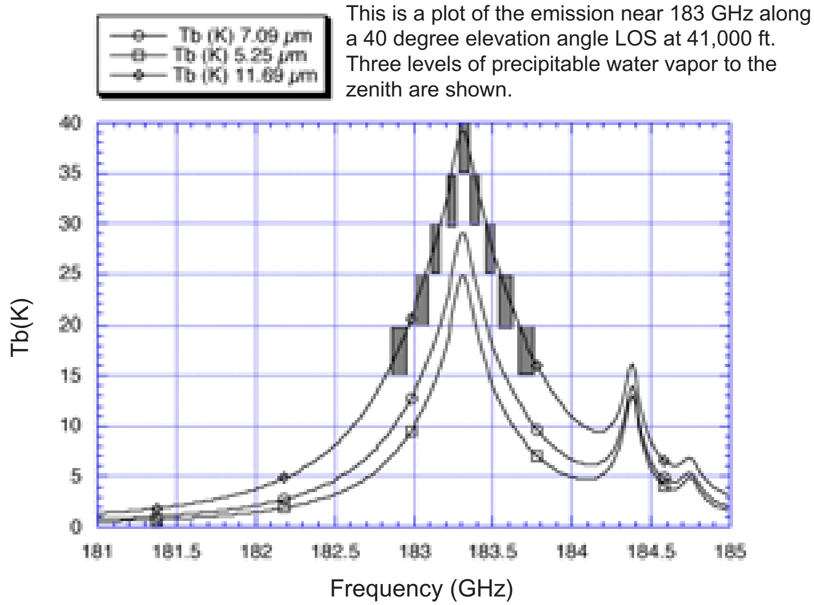

Figure 4. The 183.2 GHz water line at 41,000 ft. with three levels of water vapor. The 184.4 GHz line of ozone can also be seen. The shaded areas delineate the frequency coverage of the five double side-band water vapor monitor intermediate frequency bands.

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Spectroscopic Detection of Interstellar Organic Materials

Farid Salama, Thomas Halasinski, Bin Chen, Lou Allamandola, and Robert Walker

Understanding the origin, properties, and distribution of the biogenic elements in the universe is central to Astrobiology. The Ames Astrochemistry Laboratory has studied the ultraviolet irradiation of the molecular building blocks of interstellar and planetary organic materials. The aim of this research is to provide quantitative information to analyze astronomical spectra.

Our laboratory work has shown that polycyclic aromatic hydrocarbons (PAHs) play an important role in the interstellar medium. PAHs are complex organic molecules with the structure shown in Figure 5. Their signature is present in the ultraviolet and visible spectrum of starlight. PAHs, present as neutral, and positively negatively charged species, contain a substantial fraction (20-40%) of the organic carbon in space.

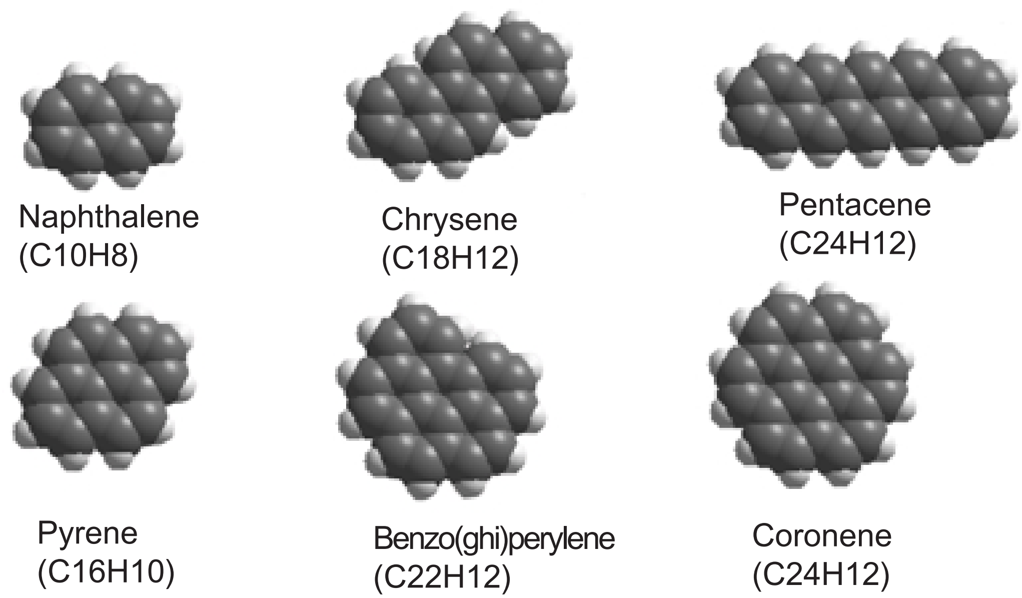

Figure 5. The three-dimensional structures of several common polycyclic aromatic hydrocarbon molecules.

Up to now, cosmic material analogs were produced in the laboratory under conditions close to, but not exactly reproducing, those expected in the interstellar medium (using cryogenic temperatures and high vacuum). The absorption and emission properties of these materials (neutral molecules and charged ions) are probed using the techniques of low temperature molecular spectroscopy. Laboratory measurements of PAHs isolated in the condensed phase (a technique called Matrix Isolation Spectroscopy) show that neutral PAHs absorb strongly in the UV. When ionized, PAHs also absorb in the visible, remarkably close to the positions of known Diffuse Interstellar Bands. Identifying the specific molecular carriers responsible for these yet unidentified bands is crucial to understand the complex organic chemistry that takes place throughout the galaxy.

There has been a great experimental challenge to measure the spectra of PAH ions in the gas phase under conditions which mimic exactly those in the interstellar medium. Within the past year, the absorption spectra of PAH cations have been measured for the first time in the gas phase using the combined techniques of Supersonic Free-Jet Expansion Spectroscopy (JES) and Cavity Ring Down Absorption Spectroscopy (CRDAS). This approach, achieved in collaboration with several research groups, allowed the first direct comparison between laboratory and astronomical data. Based on the initial laboratory results it has been concluded that a distribution of neutral and ionized PAHs represents a promising class of candidates to account for the Diffuse Interstellar Bands seen in both absorption and in emission. The results obtained so far represent a real breakthrough in astrophysics and astrochemistry as well as in molecular spectroscopy. For the first time, the absorption spectrum of a PAH cation has been measured under conditions which entirely
mimic the cold and isolated molecular ions found in the interstellar environment. ❏

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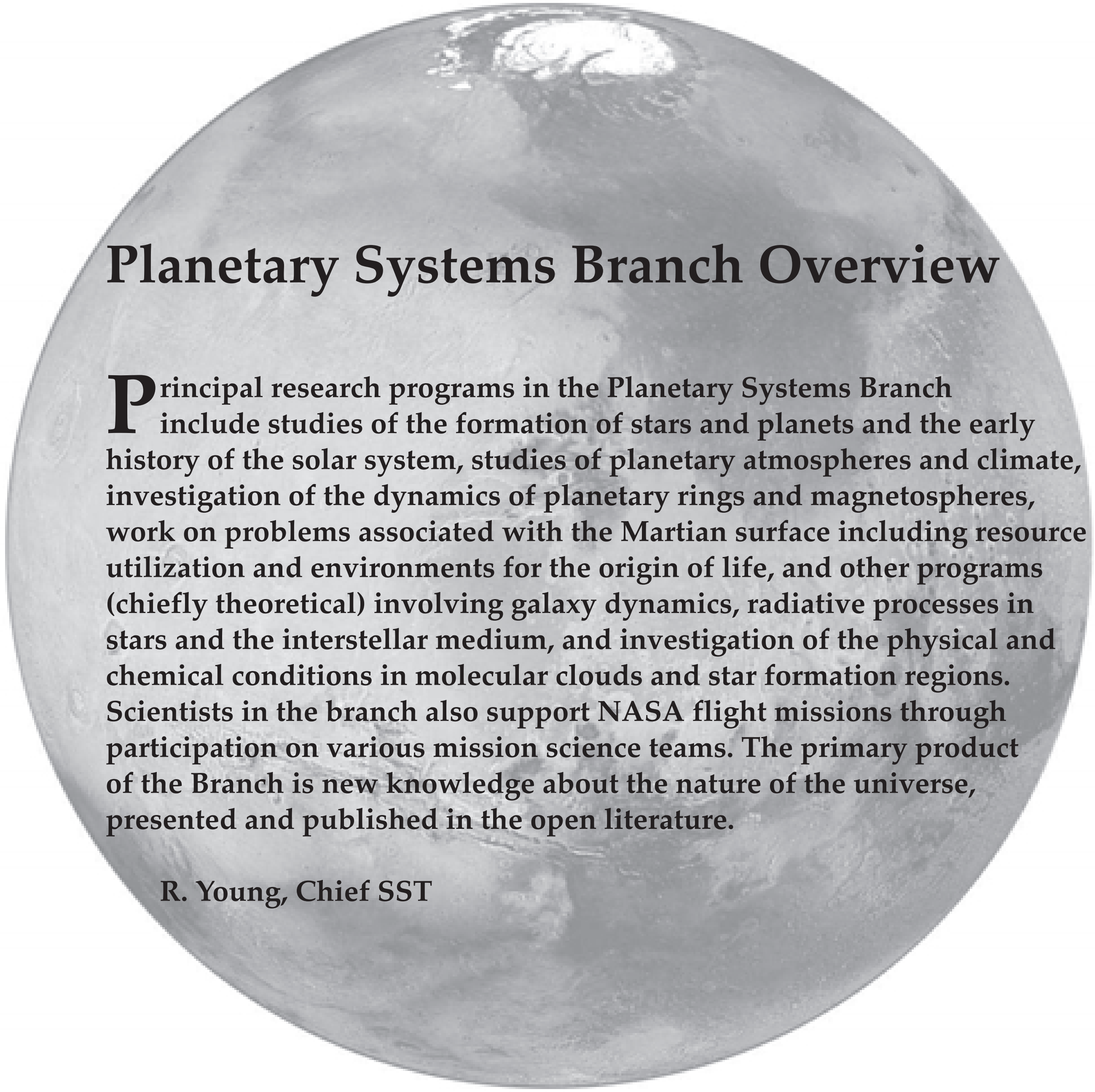

Planetary Systems Branch Overview

Principal research programs in the Planetary Systems Branch include studies of the formation of stars and planets and the early history of the solar system, studies of planetary atmospheres and climate, investigation of the dynamics of planetary rings and magnetospheres, work on problems associated with the Martian surface including resource utilization and environments for the origin of life, and other programs (chiefly theoretical) involving galaxy dynamics, radiative processes in stars and the interstellar medium, and investigation of the physical and chemical conditions in molecular clouds and star formation regions. Scientists in the branch also support NASA flight missions through participation on various mission science teams. The primary product of the Branch is new knowledge about the nature of the universe, presented and published in the open literature.

R. Young, Chief SST

Meteorites and Solar Nebula Analogs

P.M. Cassen and K.R. Bell

The planets in our solar system formed from a gaseous disk known as the solar nebula. Analogous nebulae are now commonly being observed in other solar systems by facilities such as the Hubble Space Telescope (HST) and the Infrared Astronomical Observatory (IRAS). Learning about these 'external' systems provides insight into the processes which led to the formation of our own life-supporting planetary system.

Stars typically form in dense stellar aggregates. In some clusters of young stars such as the Orion nebula, radiation from high mass stars disperses nebular material from nearby low mass systems (this process is discussed more fully in the Hollenbach *et al*. report). In many systems however, flattened nebulae, with mass sufficient to form planets similar to those found in our own solar system, survive for millions of years after the coalescence of the central star. The temperatures and densities at the midplanes of these 'protoplanetary disks' determine the characteristics of the planetary systems which ultimately arise out of the disks as well as the elemental and isotopic compositions of the meteoritic material that survived from that era. P.M. Cassen and K.R. Bell are pursuing studies of the pre-planetary evolution of solar nebula by studying analogs in external systems and the evidence in our own meteoritic record.

Until recently, purely theoretical considerations were the main source of information regarding the thermal evolution of protoplanetary disks. P. Cassen and D.S. Woolum (California State University at Fullerton) examined astronomical data regarding the photospheric temperatures of disks around T Tauri stars (young solar mass stars), as constrained by observations at optical, infrared, and radio wavelengths. They developed theoretical models to use these observations to infer the internal thermal structure of the disks. The models account for obscuring circumstellar matter, dust high in the nebular atmosphere, and the optically thick nature of the disks themselves. They found that most disks in the planet-forming stages were quite cool (at temperatures permitting the condensation of water or ice in what would correspond to the terrestrial planet region), but that disks were likely to be very hot early in their evolution, when they are still heavily obscured by in-falling material. In the latter cases, the total system luminosity provides an estimate of accretional energy. Comparisons with revealed T Tauri luminosities provide a basis for estimating the properties of embedded disks. High temperatures at early stages would explain a variety of properties characteristic of the primitive meteorites.

Evidence for nebular temperatures as deduced from meteorite properties was explored in more detail in collaborative research between K.R. Bell, P.M. Cassen, J.T. Wasson (Institute of Geophysics and Planetary Physics, UCLA), and D.S. Woolum. Patterns of elemental and isotopic abundances in meteorite components indicates that they formed in a nebula with temperatures ranging from 1400 K (above the destruction temperature of most solids such as silicates) to 400 K (a temperature low enough to permit the incorporation of water into rocky material). This wide range suggests that meteorite components were formed over an extended time during the cooling of the solar nebula. Midplane temperatures of optically visible T Tauri disks fall at the cool end of this temperature range. Using the assumption that our solar system underwent thermal evolution typical for systems with similar stellar mass, Bell et al. argued that T Tauri systems are nearing the end of their meteorite formation phases. Further, T Tauri systems must at one point have experienced a hotter, more active phase of disk evolution. This earlier phase presumably occurred while the system was still optically obscured (well embedded in the disk) and is therefore associated with the high accretion rate, protostellar phase. ❑

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Primary Accretion in the Protoplanetary Nebula

J.N. Cuzzi, R.C. Hogan, J.M. Paque, and A.R. Dobrovolskis

The 'primary accretion' of comets and asteroids is not understood. Yet, these so-called 'primitive' objects represent the parent bodies for the entire meteorite record – a vast data set that has little context for interpretation. The focus of this work is on 3D direct numerical simulations of particles in turbulence; aerodynamically-selected particles are concentrated in turbulence by a factor which can be up to a million in the nebula. Optimally selected particles have a Stokes number of unity, where the Stokes number is the ratio of particle stopping time to the Kolmogorov eddy turnover time, and is proportional to the particle radius and density. The simulation code handles Reynolds number (Re) as high as 1300, and 10^6 particles at each of 16 Stokes numbers simultaneously.

Recent results show that the shape of the turbulent concentration (TC) function is independent of both turbulent intensity (Re) and the concentration factor (in the high concentration limit appropriate for the nebula). The predictions are well-fit by a lognormal function. Also, a so-called 'unequilibrated ordinary chondrite' ALH 85033 was 'disaggregated' and the size distribution of the chondrules was measured directly. These data are far superior to similar data obtained by examining slices of rock in a microscope; they provide direct determination of the chondrule density, which cannot be attained any other way. Previous research merely measured particle radius and assumed an average density for all particles. The new data change the shape of the distribution curve for concentration.

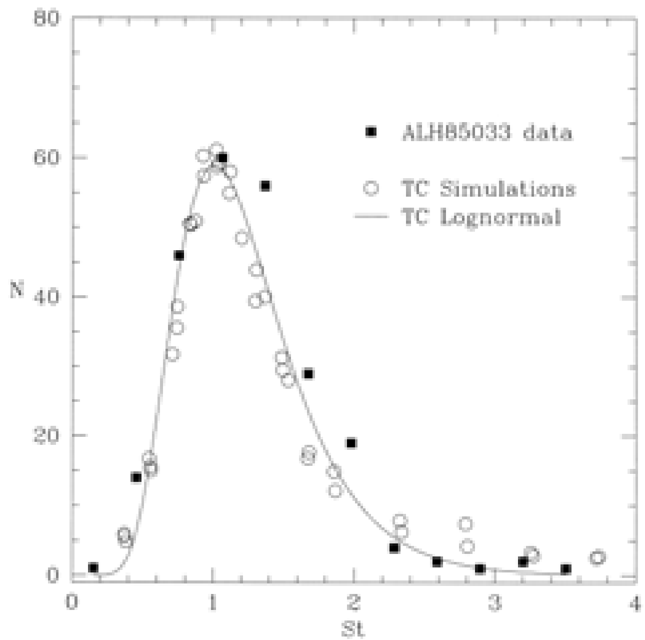

Figure 6. Comparison of model predictions with the actual relative abundance of chondrules, as a function of the product of particle radius and density.

Figure 6 compares model predictions with the actual relative abundance of chondrules, as a function of the product of particle radius and density. The open circles are the predictions, for all three Re values we simulated – there is no significant Re dependence of the shape.

The solid curve is the best fit of a lognormal function to the actual simulations. The filled squares are the meteorite data. The data and the predictions are normalized together at their peaks, and the shapes agree very well without any free parameters in the theory. The so-called Weibull function previously assumed (also shown) is based not on aerodynamic sorting but on fracture processes, and has several free parameters.

The theory was also generalized to other particle properties and nebula locations. Not all particles in the nebula are likely to be solid silicates. The earliest condensate grains probably stick into fluffy 'fractal puffballs' and then porous aggregates which have lower average density. These particles will incur preferential concentration in areas of the nebula where the gas density is commensurately lower, such as the formation regions of the gas giants and comets.

Figure 7 shows the expected particle radius-density product amenable to preferential concentration as a function of turbulent intensity (the latter expressed as scaling parameter alpha). Current estimates for nebula alpha are in the range from 10^{-4} to 10^{-2}. Thus, while solid chondrules (CH) are concentrated in the terrestrial planet region (1-2.2 AU, or astronomical units, where 1 AU is the earth's distance from the sun), porous aggregates (PA) are concentrated at the same level of turbulence in the lower density regions at the locations of Jupiter, Saturn, and Uranus (5, 10, and 20 AU). Low gas density is also found at large heights above the nebula midplane even at 1-2 AU. The most fluffy aggregates (FA) are concentrated at extremely low density and/or high turbulent intensity. ❑

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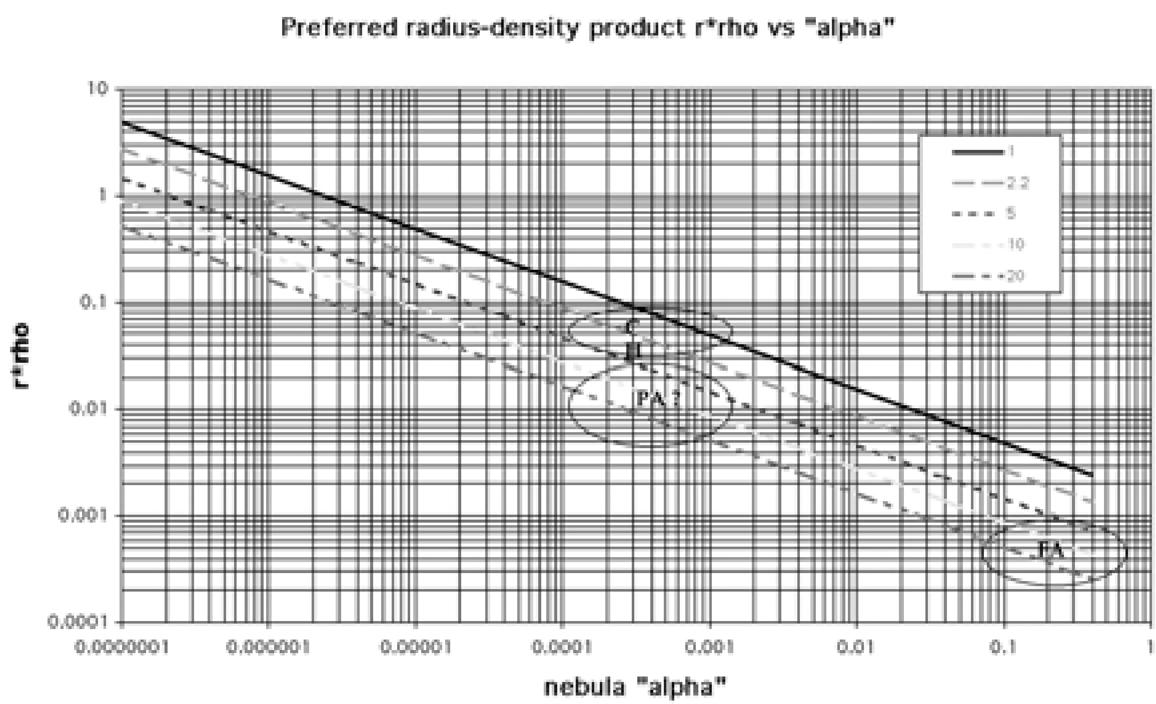

Figure 7. The expected particle redius density product amenable to preferential concentration as a function of turbulent intensity.

The Center For Star Formation Studies

D. Hollenbach, K.R. Bell, and P. Cassen

The Center for Star Formation Studies, a consortium of scientists from the Space Science Division at Ames and the Astronomy Departments of the University of California at Berkeley and Santa Cruz, conducts a coordinated program of theoretical research on star and planet formation. The Center, under the directorship of D. Hollenbach (NASA Ames), supports postdoctoral fellows, senior visitors, and students, meets regularly at Ames to exchange ideas and to present informal seminars on current research, hosts visits of outside scientists, and conducts a week-long workshop on selected aspects of star and planet formation each summer.

One focus of the NASA Ames portion of the research work in 1998 involved the dispersal of the protoplanetary disks which ultimately form planets. The formation of a planetary system includes a number of sequential stages. The collapse of a giant cloud of interstellar gas and dust results in a central protostar with a protoplanetary disk of orbiting gas and dust. The gas and dust spirals onto the star, causing the star to grow in mass, a process called 'viscous accretion.' At the same time, the dust in the disk settles to the midplane, and coagulates into large, ice/rock planetesimals. The collisions of these planetesimals leads to larger planets, and if the mass of the planet becomes greater than about 15 Earth-masses, the gravity of the planet can attract the gas in the disk, and the planet rapidly adds considerable more mass as it accretes gaseous hydrogen and helium. In this way, giant gaseous planets such as Jupiter are formed. During the same period, the wind from the central star 'blows' on the disk and carries gas and dust back out into the interstellar medium. In addition, the ultraviolet radiation from the central star, or from a nearby, luminous star, heats the surface of the disk to thousands of degrees in temperature, and the gas and dust is evaporated into the interstellar medium. Therefore, the gas and dust in a protoplanetary disk have four possible fates: accretion onto the star, accretion onto planets, wind-stripping, or photoevaporation. D. Hollenbach, H. Stoerzer, D. Johnstone (University of Toronto), and H. Yorke (Jet Propulsion Laboratory) studied the relative importance of these four disk dispersal mechanisms. They showed that winds are probably not significant, and that the photoevaporation and viscous accretion mechanisms compete with planet formation in dispersing the disk in a time scale on the order of one to ten million years. The outer disk is especially susceptible to photoevaporation, and this may explain why Uranus and Neptune have so much less gas mass than Jupiter and Saturn. Many planetary systems form in clusters which include massive, luminous stars. The ultraviolet radiation from these luminous stars can evaporate their own disks, and nearby disks circling lower mass stars, in time scales of order 100,000 to 1,000,000 years, perhaps preventing or truncating planet formation.

Disks observed around low mass young stars, which are not disrupted by nearby bright stars, are expected to give rise to planetary systems. Research by P.M. Cassen and D.S. Woolum (California State University at Fullerton) has led to a derivation of disk midplane conditions from observations of disk around young, low mass systems (see the Cassen and Bell report for more details on this research). They find that disks in the planet-forming stage are quite cool. They, along with K.R. Bell and J.T. Wasson (Institute of Geophysics and Planetary Physics, UCLA), argue from meteoritic abundance patterns that an earlier, hotter phase of nebular evolution must have existed. This phase is identified with embedded protostars.

The theoretical models developed by the Center have been used to interpret observational data from such NASA facilities as the Infrared Telescope Facility (IRTF), the Infrared Astronomical Observatory (IRAS), the Hubble Space Telescope (HST), and the Infrared Space Observatory (ISO, a European space telescope with NASA collaboration), as well as from numerous ground-based radio and optical telescopes. In addition, they have been used to determine requirements on future missions such as the Stratospheric Observatory for Infrared Astronomy (SOFIA) and the proposed Space Infrared Telescope Facility (SIRTF). ❏

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Detection and Models of Extrasolar Planets

Jack J. Lissauer

The objectives of this project are to study planets around stars other than our own Sun both observationally and by developing theoretical models of the formation and stability of planets and planetary systems.

A team of astronomers from San Francisco State University, the Anglo-Australian Observatory, Lick Observatory, and Ames have discovered a planetary-mass companion orbiting the star Gliese 876. The newly found body has a mass multiplied by the sine of the inclination of its orbit normal to the line of sight of 1.9 times that of Jupiter, a period of 61 days (implying a semi-major axis of 0.2 AU) and an eccentricity of 0.37. The planet was identified using Doppler measurements of the radial velocity of the star at the Keck and Lick observatories. This planet is closer to the Sun than is any other extrasolar planet thus far identified. More significant is the fact that Gliese 876 is an M4 star with a mass about 1/3 that of our Sun. This is the first planet to be discovered in orbit about an M star, and as most stars in our galaxy are faint M stars like Gliese 876, its existence suggests that billions of planets probably are present within our galaxy.

A set of plausible outer planetary systems were constructed using direct numerical integrations by a team of astronomers from the Southwest Research Institute, Queen's University, and Ames. It was found that in order to construct planetary systems like our own, some sort of dissipation was required to continue during the accretionary epoch for time scales longer than 10 million years. The number of planets can vary from one to seven. Systems with a large number of planets never contain very massive, Jupiter-like planets, but instead are made up of Uranus-like planets. Stable planetary systems can include planets in mean motion resonances with one another. Perhaps most surprisingly, it is possible to construct stable systems in which planetary orbits can undergo large, semi-periodic changes.

Models of the growth of giant planets close to their stars were constructed by a group from Lick Observatory and Ames. If adequate solid planetesimals are available near stars, planetary cores can grow massive enough to accrete large amounts of gas from the protoplanetary disk. However, for conditions similar to those believed to have existed around our Sun, planetary growth several astronomical units from the star, followed by subsequent inward migration, appears to offer a more likely scenario. ❑

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1999 Marsokhod Rover Field Experiment

C. Stoker, N. Cabrol, T. Roush, J. Moersch, V. Gulick, G. Hovde, and the Marsokhod Rover Team*

A field experiment to simulate a rover mission to Mars was performed in Feb. 1999. This experiment, the latest in a series of rover field experiments, was designed to demonstrate and validate technologies, investigate strategies for high-science, high-technology performance, and define cost-effective planetary rover operations.

The experiment objectives were to: 1) train scientists in a mission configuration relevant to Mars Surveyor program rover missions at a terrestrial analog field site simulating the criteria of high-priority candidate landing-sites on Mars; 2) develop optimal exploration strategies; 3) evaluate the effectiveness of imaging and spectroscopy in addressing science objectives; 4) assess the value and limitation of descent imaging in supporting rover operations; and 5) evaluate the ability of a science team to correctly interpret the geology of the field site using rover observations.

A field site in the California Mojave Desert was chosen for its relevance to the criteria for landing site selection for the Mars Surveyor program. These criteria are: 1) evidence of past water activity; 2) presence of a mechanism to concentrate life; 3) presence of thermal energy sources; 4) evidence of rapid burial; and 5) excavation mechanisms that could expose traces of life.

The Marsokhod rover shown in figure 8 was used for the test. The Marsokhod chassis is an all-terrain vehicle developed as a flight

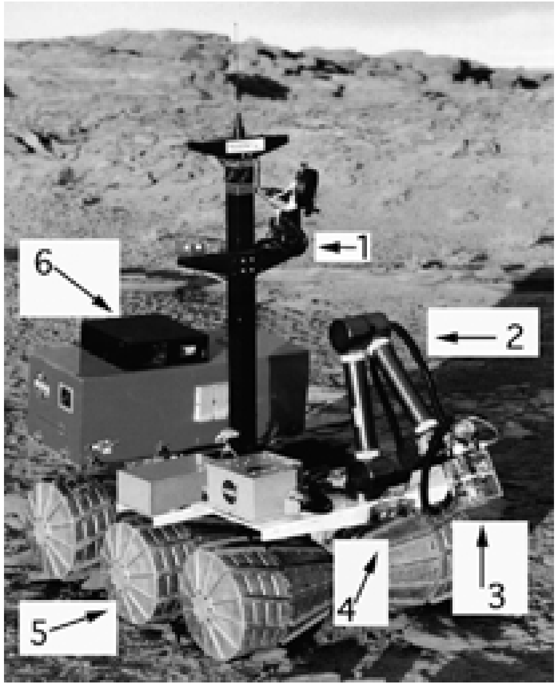

Figure 8. Marsokhod rover with: 1) mast carrying stereo color cameras, stereo navigation cameras and NIR spectrometer; 2) five DOF manipulator arm; 3) carousel end-effector; 4) front pallet navigation cameras; 5) titanium wheels; 6) onboard electronics and computer.

prototype by the Mobile Vehicle Engineering Institute (VNIITransmash) in Russia. The chassis is 100-cm wide, 50-cm long, and has a 35 kg unloaded mass. The chassis consists of three pairs of independently driven titanium wheels, joined together by a three degree-of-freedom (DOF) passively articulated frame. Two degrees-of-freedom allow the frame to twist, while the third allows it to pitch. The central mast carries a stereo imager consisting of two 3-chip color 640x480 pixel CCD cameras providing 0.30 mrad/pix resolution with a 25-centimeter stereo baseline at 178-cm height. Monochrome stereo CCD cameras with resolution of 0.9 mrad/pix are mounted on the mast and the front and rear pallets near the wheels. These cameras are used for navigation and arm placement.

The rover payload also includes a Near Infrared (NIR) fiber-optic spectrometer operating in the range from 0.35 to 2.5 micrometers. The 1 degree instrument field of view (IOFV, approx. 17 mrad) fore-optic of the spectrometer is bore-sighted with the color stereo mast camera. The files produced by the spectrometer are automatically interpolated by the data collection software from the nominal instrumental spectral resolution to a resolution of 0.001 micrometer over the entire spectral domain. Automated spectral analysis was performed onboard to search for the spectral signature of carbonate minerals. Finally, the Marsokhod was equipped with a 5 DOF manipulator arm and a carousel end-effector. A color camera mounted on the end-effector of the arm could resolve 0.08 mm/pixel at closest position. A clamshell scoop occupied another position in the carousel.

Some additional instruments were included as part of the simulated payload but were operated independently from Marsokhod. A set of simulated descent images were obtained using a helicopter flight over the landing site. The image resolutions and field of view were designed to simulate the Descent Imager camera selected for the 2001 Surveyor mission. A portable, battery-powered Fourier transform infrared (FTIR) spectroradiometer operating in the 8-14 µm wavelength range at a resolution of 6 cm^{-1} simulated the Thermal Emission Spectrometer selected for the Mars 2001 mission. A foreoptic gives an IFOV of 15 mrad (FWHM), or 15 cm at a range of 10 m. This spectrometer, mounted on a tripod, was pointed by a field assistant at targets specified by the science team. Finally, simulated arm camera images were obtained with an engineering model of the University of Arizona Robotic Arm Camera selected for flight on Surveyor Mars missions for 1998 and 2001. This instrument was mounted on a tripod and pointed by a field assistant upon commands from the science team. It was used to image the walls of a trench dug by a field assistant.

Twenty participating scientists, unfamiliar with the site, directed the rover science mission for two weeks in February 1999. Prior to the mission, the science team were provided with orbital images with resolutions comparable to Viking and MOC images, and with Landsat Thematic Mapper images to use for traverse planning and formulating a science strategy. Simulated descent images were provided to the science team at the outset of the rover operations. A portable satellite dish, set up at the field site, enabled communication between mission control at Ames Research Center and the rover in the field. Data volumes were restricted to 40 mbits per command cycle as expected for actual Mars Surveyor missions. During the primary phase of the mission (Feb. 8-10, 1999) a total of 3 communication cycles/day were used by the science team located at Ames. During the extended phase of the mission, 1-2 cycles/day were used and the science team, many of whom participated from their home institutions via a world-wide-web interface and teleconferences. The science team was asked to: 1) use the orbital and descent data to develop hypotheses that could be tested using rover data; 2) characterize and identify rocks representative of the main geological events at the landing site; 3) identify the main geologic processes that have operated on materials at the landing site using their mineralogy, surface texture, morphology, and context; 4) reconstruct the stratigraphic sequence of events at the landing site; 5) identify rocks and soils that have the highest chance of preserving ancient environmental conditions favorable to life; and 6) characterize and cache samples of rocks which may have preserved evidence of life. Science team interpretations were compared with ground truth as evaluated by a science team in the field.

* Marsokhod Rover team is the staff of NASA Ames Intellegent Mechanisms Group and other members of the Information Technology Division at NASA Ames Research Center. ❏

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Magnesium-Rich Pyroxene Crystals Discovered in Comet Hale-Bopp

Diane Wooden

Analysis of silicate features in comet Hale-Bopp led to the discovery of abundant magnesium (Mg)-rich pyroxene crystals in the coma. Hale-Bopps' pyroxene crystals are analogous to pyroxene Interplanetary Dust Particles (IDPs), which also may be of cometary origin. The Mg-rich pyroxene crystals represent either pristine solar nebula condensates or relic interstellar grains. If the Mg-rich pyroxene crystals are relic interstellar grains, their preponderance in cometary comae implies that the outer solar nebula, where icy planetesimals formed, received significant contributions of presolar materials. Interstellar relic grains in comets are probable sources of complex organic molecules. Such complex organic materials may have been delivered by comets to early Earth during the heavy bombardment period.

The Ames HIFOGS mid-IR spectrometer acquired 7.5-13.5 µm spectra of comet Hale-Bopp over a large range of heliocentric distances from July 1996 through August 1997. Silicate minerals produce Si–O vibration modes in this portion of the electromagnetic spectrum. Comet Hale-Bopp was observed over a large range of heliocentric distances (3.6 AU to 0.95 AU, and back out to 2.4 AU) and the silicate feature was discovered to change in shape as the comet approached the Sun, and revert to its previous shape upon recession from the Sun. From analysis of the temporal evolution of these mid-IR spectra, a cooler, Mg-rich crystalline silicate grain component – crystalline pyroxene (Mg, Fe) SiO_3 – was discovered in the comet. The pyroxene crystals are so

Mg-rich that they absorb sunlight less efficiently, making them cooler than the other silicate mineral grains. These pyroxene crystals are about ten times more abundant than the other silicate grains, and have been previously spectroscopically undetected in comets. The preponderance of Mg-rich pyroxene crystals in comet Hale-Bopp agrees with the dominance of pyroxene IDPs and with the dominance of Mg-rich pyroxenes in the reanalysis of PUMA-1 flyby measurements of comet Halley. ❏

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Refugia from Asteroid Impacts on Early Mars and Earth

Kevin Zahnle and Norman H. Sleep

Impacts on planets by large comets and asteroids were relatively frequent events in the early solar system. These impacts posed a major recurrent hazard to the continuous existence of life on early Mars and Earth. The chief danger would have been presented by globally distributed ejecta. These ejecta included large sub-orbital projectiles, mountains of finely subdivided dust, and in the worse case thick transient rock vapor atmospheres. On the Earth, down-welling thermal radiation from the hot atmosphere boiled the surfaces of the oceans. Water evaporated until either the energy contained in the rock vapor atmosphere is exhausted or the oceans boiled off. The Earth's oceans thereby provided an enormous thermal buffer that limited thermal excursions triggered by very large impacts, provided that the impact was not too large. Life could have survived in deep cool waters or in deep subsurface 'hideouts' until the danger passed and the rock was returned to its desirable crustal status. But if an impact was truly enormous (>1028 Joules, or a 500-km-diameter impactor 'the size of Texas'), the oceans vaporized and it would take at least 3000 years, (the time required to recondense and rain out all the water of the oceans) for conditions to return to some semblance of their original state. Thermal conduction would carry the thermal pulse to some considerable depth, while upwelling geothermal heat (much more than experienced in modern times) would leave any habitable niches wedged 'between the firepan and the fire.' Under such conditions the survival of any life present on the Earth would be threatened.

The lack of deep oceans on Mars means that there is no thermal buffer against even relatively small impacts and so the effect is quite different. Even an impact as small as the K/T event (the Cretaceous/Tertiary asteroid that killed the dinosaurs and 95% of the other lifelines on the Earth) would raise the martian surface to the melting point. This would be bad for life at the surface (e.g., for photosynthesizers), but the melting would not be deep, and the effects would soon (i.e., in hours-to-days) be forgotten as the energy of the impact quickly radiates into space. Even for larger events, the effects, although briefly scalding, are mitigated on Mars. For example, the low martian escape velocity permits a fair fraction of the hottest and most energetic ejecta to escape entirely, and thus not contribute to hazards to the hypothetical biota. Instead, because the gravity is lower the global ejecta on Mars are relatively massive but relatively cool. Survival of subsurface ecosystems is more likely on Mars than on Earth because: 1) Mars' lower geothermal heat flow and lower gravity permit deeper colonies (it is gravity that crushes rocks and seals pores; lower gravity permits deeper circulation of fluids, etc.), and 2) The thermal pulse from a major impact is more brief, thus there is more space between the firepan and the fire.

The possibility that Mars may have provided a more survivable platform for life in the earliest solar system, coupled with the demonstrated fact that Earth at least can receive lightly shocked ejecta from Mars, brings us to consider briefly the implications of exchange of materials between the two worlds. Lightly shocked ejecta, launched by impact and possibly stocked by crews of inadvertent microbial spacefarers, could make the voyage between planets. It does seem possible, even likely, that viable organisms have been launched by impact on favorable trajectories from Earth to Mars, so that after a relatively brief and altogether survivable trip through interplanetary space the terrenes might have found suitable homes; and of course the story could be reversed, which would make us all, in a sense, martians. ❏

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Martian Oxidant Mixing by Impacts

Aaron P. Zent

It is the objective of this work to revise previously published profiles of the oxidative stratigraphy of the martian regolith to include the effects of regolith stirring by impact cratering. The fundamental objectives are to estimate the depth from which samples must be obtained in order to access martian organics, and to clarify the unknowns in the problem to help direct future research.

One of the fundamental operational objectives of NASA's Exobiology Program is to return and examine organic material from the martian regolith. This objective derives from observations of the martian surface that indicate liquid water played an as-yet-unexplained role in the evolution of the martian surface early in the planets history, the same period during which life is suspected to have made its first appearance on Earth. The chemical evolution that lead to terrestrial life might have occurred on Mars as well The opportunity to compare the paths of prebiotic chemical evolution on two planets is likely to illuminate fundamental principles that govern the abiotic origin of life.

The most salient barrier to this objective is that the martian regolith is highly oxidizing, thus destroying putative martian oxidants. The specific chemical mechanisms which are responsible for the oxidizing nature of the martian surface remain unknown, but the photochemistry of atmospheric water is thought to be the ultimate source of the oxidants). This hypothesis predicts that strong oxidants are present at the base of the martian atmosphere and diffuse into the martian regolith, where they can react with any organics that may be at depth. The depth to which the oxidants might diffuse is unknown, but the regolith sampled by Viking was found to be oxidized to 10 mm. Therefore, considerable effort is being expended to understand the adsorptive and diffusive properties of H_2O_2 through silicate materials, as well as their reaction and complexation pathways, so that the thickness of the oxidizing layer can be predicted. However, it may not be sufficient to understand the diffusion of a vapor phase oxidant into the martian regolith, because the martian stratigraphic column is not stable, and was even less so early in its history. Aeolian and impact mechanisms act to erode and deposit material across the martian surface, effectively stirring the surface materials.

It is possible to estimate quantitatively, the mixing of a near-surface oxidized layer into the martian subsurface by impact cratering. Impact craters leave a clear signature in a planetary surface. Mixing models can be constructed (see figure 9) based upon simplified geometric and probability assumptions, which will describe the movement of materials up into the oxidizing zone, and down again, in response to subsequent burial (this cycling of material is referred to as 'regolith gardening.')

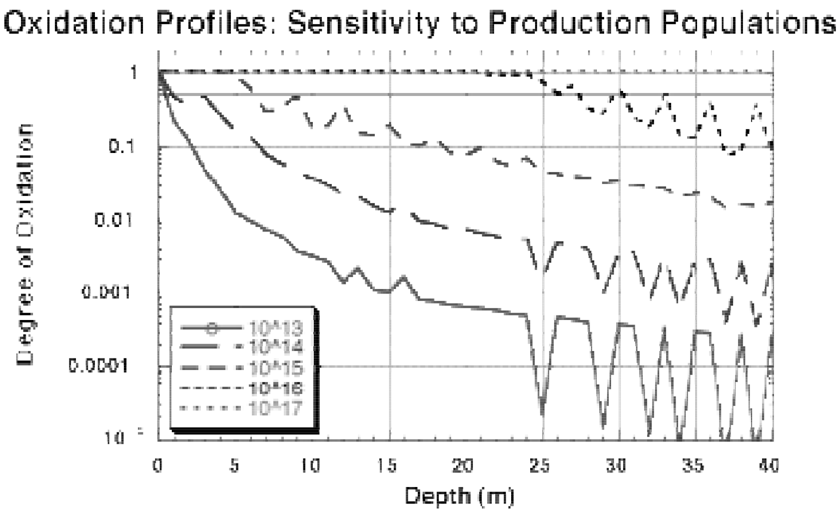

Figure 9. The sensitivity of the regolith oxidation profile to the pre-exponential factor in the production population is shown in this plot. Each increase in a factor of 10 in impact frequency considerably increases the depth from which samples must be acquired. The horizontal line represents a 50% likelihood of retrieving putative organics.

The effects of regolith gardening are quantitatively estimated, and combined with the effects of oxidation by atmospheric gases to produce estimates of the degree of oxidation of the martian surface with depth. We explore the effects of different crater production populations along with variations in H_2O_2 extinction depths, and hydrothermal oxidation of ejecta. In very select circumstances involving very early onset of oxidizing conditions during heavy bombardment, 150 to 200 m of regolith could be fully oxidized. More likely scenarios for the crater production population, onset of oxidizing conditions, and oxidant extinction depth yield estimates of no more than a few meters to putative reducing material. In addition, uncertainties remain regarding the degree to which hydrothermal or other high temperature chemistry might oxidize materials in ejecta blankets. The trade between accessing unlithified sediments or rock interiors must be considered. ❑

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Exobiology Branch Overview

Research in the Exobiology Branch focuses on the advancement of the scientific understanding of the origin and distribution of life by conducting research on the cosmic history of biogenic compounds, prebiotic evolution, and the early evolution of life. This is accomplished via laboratory experiments, theoretical studies/computational modeling, and field investigations. Branch personnel are also involved in the development of flight instruments, experiments, and small mission definition with particular emphasis being placed on studies of Mars and the development of instrumentation for martian flight missions. Several Branch scientists are part of a task module that is part of the Ames membership in the Astrobiology Institute. Branch scientists provide expertise in exobiology, astrobiology, planetary protection, and other areas of planetary science to NASA Headquarters and external review and advisory panels, and some serve as editors and associate editors of scientific journals.

M. Fonda, Chief SSX

The Ecology of Modern Microbial Mats and Stromatolites

Brad Bebout, Pieter T. Visscher, and Jack Farmer

Work in the Microbial Ecology/Biogeochemistry Research Lab focuses on characterizing the biological activity of microbial mats and stromatolites. This is accomplished using a combination of field and laboratory studies of modern microbial mat and stromatolite communities. Microbial mats (laminated microbial ecosystems occurring in a variety of aquatic environments) and stromatolites (which can be thought of as mats in which minerals are being trapped and/or precipitated) are modern examples of the most ancient biological communities on Earth, examples of which are preserved in rocks as old as 3.5 billion years.

Mineral formation in microbial mats, which occurs to make stromatolites, is important to understand as it is primarily the stromatolites, and not the microbial mats, which become a part of the fossil record of life on Earth. Particular key questions being addressed are: What are the conditions under which these mat communities actually 'turn to stone'? What happens to the organisms building the community as this happens? What are the biological consequences? In collaboration with a team of scientists led by R. Pamela Reid (University of Miami) and funded by the National Science Foundation, studies of stromatolites found in the Bahamas have resulted in a model of one set of processes leading to lithification (formation of rock).

Trace gas production and consumption in microbial mats is important to understand for a number of reasons. In addition to representing a potential loss of organic matter by the community, these gases diffuse into the atmosphere, where they can affect climate (as in the case of dimethyl sulfide and methane). In addition, the detection of some of these gases in the spectra of atmospheres of extrasolar planets is considered to be a viable search strategy for the detection of life on extrasolar planets. Biological processes within these communities control the amounts and timing of the release of various trace gases. The trace gases produced and consumed by microbial mats from various environments have been quantified, and some of the factors affecting these rates of production consumption have been identified.

Technology development in the lab has centered on finding better ways of measuring rates of metabolic processes, the concentrations of biologically important chemical species, and the rates of production and consumption of trace gases in situ (in the natural environment). Naturally occurring microbial mats and stromatolites are subjected to conditions of water flow, temperature, and sunlight which are difficult, if not impossible, to simulate in the laboratory. Extensive fieldwork in Yellowstone National Park, the Bahamas, and Baja California, Mexico has therefore been undertaken. Preliminary versions of a device designed to make in situ measurements of oxygen concentrations within these communities at 100-micrometer spatial resolution were tested and evaluated. New types of sensors designed to measure the light available for photosynthesis within these communities are also under development. A new device designed to measure the degree of lithification (as hardness) within stromatolites was developed and tested in the Bahamas. ❏

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Evaluation of Evidence of Life in the Martian Meteorite ALH84001

David Blake, Sherry Cady, Kannan Krishnan, and Allan Treiman

In 1996, an announcement was made that fossil evidence of bacterial life had been found in a meteorite known to have originated from Mars. One of the main lines of evidence for the putative bacterial fossils in the Martian meteorite ALH 84001 is the presence of submicroscopic crystals of the mineral magnetite that are similar in size and shape to biogenic magnetite crystals formed by primitive bacteria on Earth. The terrestrial organisms, called magnetotactic bacteria, use the magnetite to navigate in the Earth's magnetic field. While some bacterial species are able to mediate the deposition of minerals in the local extracellular environment, magnetite from terrestrial magnetotactic bacteria is known to be formed only within the cell membrane of the bacterium. In ALH84001, the submicroscopic magnetite is found in large aggregations associated with iron- and magnesium-rich carbonates, and the supposition is made that the magnetite survived the demise of the organisms and was passively incorporated into the surrounding carbonate. In this report, new evidence is presented concerning the ALH84001 magnetite which points to an inorganic origin.

This work utilized a petrographic thin section of the meteorite, obtained from the curatorial collection at Johnson Space Center. Small portions of the meteorite material which contained both carbonate and magnetite were removed from the thin section and attached to electron microscope sample grids. The grids were placed in a sample preparation device which milled the material to a thickness less than 0.1 µm (one ten millionth of a meter, or about 1/1,000 the diameter of a human hair). The thinned material was viewed in a high resolution Field Emission Transmission Electron Microscope (FETEM) at the

National Center for Electron Microscopy, Lawrence Berkeley Laboratories. In the FETEM, magnifications are achieved in which planes of atoms making up the magnetite and carbonate crystal structures can be directly viewed.

At high magnifications, the relationship of the magnetite crystal structure to that of the carbonate crystal structure is apparent. Figures 10a-b, for example, show a high-resolution image of a single crystal of magnetite within the carbonate matrix. The fine lines in 10b are

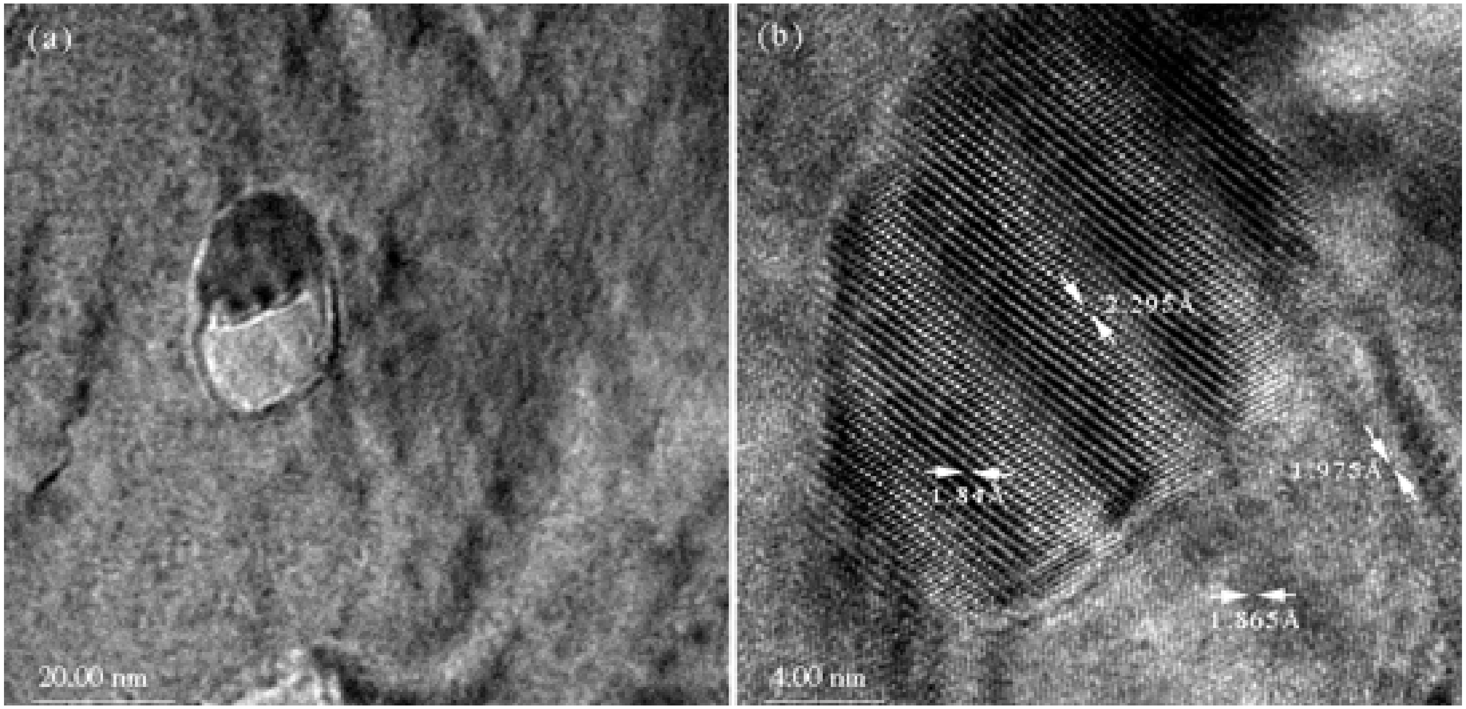

Figure 10. High-magnification images of magnetite in epitaxial orientation to enclosing carbonate. (a) view of a single magnetite crystal enclosed within a small hole in the carbonate. (b) Lattice-resolution image of the magnetite and carbonate shown in (a). Atomic planes in the magnetite have closely similar spacing and parallel orientations to those in the carbonate, typical of an epitaxial relationship. The likelihood that this orientation occurred randomly after the magnetite was formed (e.g., within a bacterial cell) cannot be entertained.

planes of atoms making up the crystal structures of the carbonate and magnetite phases. One can see that certain planes of atoms or crystallographic directions within the magnetite structure are in alignment and have spacing similar to planes of atoms, or crystallographic directions of the surrounding carbonate. A significant number of magnetites was found to be related to the surrounding carbonate in this way. This preferred orientation, which is called epitaxy, is proof that the magnetite nucleated and grew on the surrounding carbonate. If the magnetite nucleated and grew at a site removed from direct contact with the carbonate (for example, within the membrane-bound body of a bacterial cell) and was later deposited in the carbonate, it would be highly improbable that such a special orientational relationship would arise.

Not all magnetite exhibits an epitaxial relationship with the surrounding carbonate within ALH84001. However, it is highly unlikely that magnetite crystals which do not exhibit epitaxy but which occur in identical spatial and temporal settings within the meteorite, were formed by an entirely different mechanism. Indeed, evidence obtained by Ames researchers suggests that the magnetite was precipitated inorganically from a carbonate-rich hydrothermal solution. The presence of nearly identical spacing between atomic planes in the carbonate and magnetite phases facilitates nucleation of the magnetite onto the carbonate from sparingly saturated hydrothermal solutions. Epitaxial growth of one phase on another avoids the activation energy barrier associated with homogeneous nucleation, a significant hindrance to crystallization in most systems. During continued crystallization, a level of supersaturation must have been achieved in which magnetite could precipitate directly from solution without the requirement for a precursor phase.

Evidence now points to an inorganic origin for many of the features reported from the ALH84001 meteorite. However, analyses of the meteorite do suggest that carbonate-rich hydrothermal solutions existed in the near-surface environment on Mars 3.9 billion years ago, around the time that the first evidence of life is found on the Earth. It remains that Mars is one of the most interesting objects in the solar system from an Astrobiological point of view, and evidence of hydrothermal systems and carbonate deposition in the early wet and warm period of Mars history only increases our interest in that planet. ❏

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Progress on a Laboratory Version of CHEMIN, An X-Ray Diffraction X-Ray Fluorescence Instrument

David Blake, Philippe Sarrazin, David Bish, David Vaniman, and Stewart A. Collins

CHEMIN is a miniaturized Charge Coupled Device-based (CCD) X-ray diffraction/X-ray fluorescence (XRD/XRF) instrument. The name CHEMIN refers to the instrument's combined CHEmical and MINeralogic analytical capability. The instrument, for which a patent was awarded to NASA in 1996 ("X-ray diffraction apparatus," US Pat. No. 5,491,738) is designed to characterize the major element composition and mineralogy of small fine-grained or powdered samples. Both diffraction and fluorescence data are obtained simultaneously by exposing a 2-dimensional CCD imager directly to the X-rays and sorting out the photons according to their energies. CHEMIN was originally designed as a spacecraft instrument, and has been proposed for five flight missions including most recently the Mars 2001 opportunity. However, during the development and characterization of the flight instrument, it was found that CHEMIN was superior in many ways to the laboratory instruments from which it was derived. The CHEMIN design team has recently begun adapting the flight instrument for use in terrestrial laboratories and in remote locations on the Earth.

There are several aspects of the design that make the instrument ideal for certain types of laboratory analysis. CHEMIN is the first combined XRD/XRF device for which data of both types are recorded concurrently from the same micro-area of the sample. Areas as small as 30 micrometers in diameter can be analyzed using conventional laboratory X-ray sources. The CCD detector is 2-dimensional, allowing for detection of the entire front reflection region of the diffraction pattern, from the primary beam direction to nearly 60 degrees in 2-theta space. This results in a nearly 2-order of magnitude improvement in counting rate over conventional X-ray diffractometers. In addition, because full debye rings are collected, one can record fully quantitative data from as-received or poorly prepared materials. Preferred crystal orientation and variation in crystallite size, important parameters in geology, biology, and materials science can be assessed directly using CHEMIN.

Because the CCD detector can discriminate X-ray photons according to their energies, several diffraction patterns can be collected at once, using different X-ray source energies. This allows concurrent collection of data from large 'd-value' materials such as clays at the same time as small d-value materials such as ceramics. The real-time nature of data collection will allow researchers to follow the course of reactions or phase changes using X-rays in much the same way that

Fourier Transform Infrared Spectroscopy is performed today. The CHEMIN laboratory instrument is equipped with a miniaturized (about the size of a pencil stub) low-power micro-machined field emission X-ray source developed by MOXTEC, Inc. as a Small Business Innovative Research (SBIR) project. An advanced CCD with improved X-ray energy resolution, developed by Jet Propulsion Laboratories for an astrophysics mission will be used as a detector for the instrument. X-ray diffraction data are recorded (in transmission mode), for atomic spacings from 1.66 to 15 Ångstroms, a range which covers definitive maxima for nearly all minerals (see, for example figures 11 and 12).

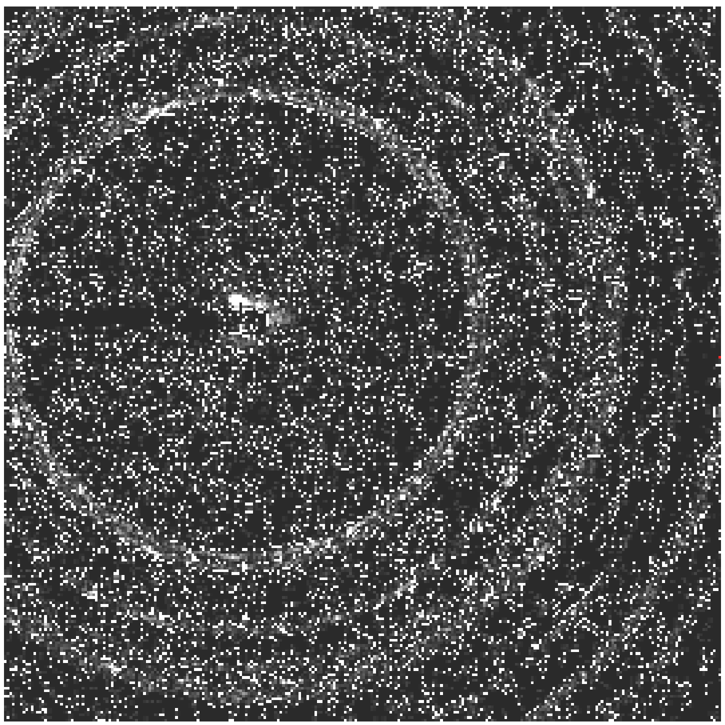

Figure 11. Diffraction pattern for Aragonite, $CaCO_3$ using an unfiltered copper X-ray source. The pattern is comprised of monochromatic copper K photons, chosen according to their energy.

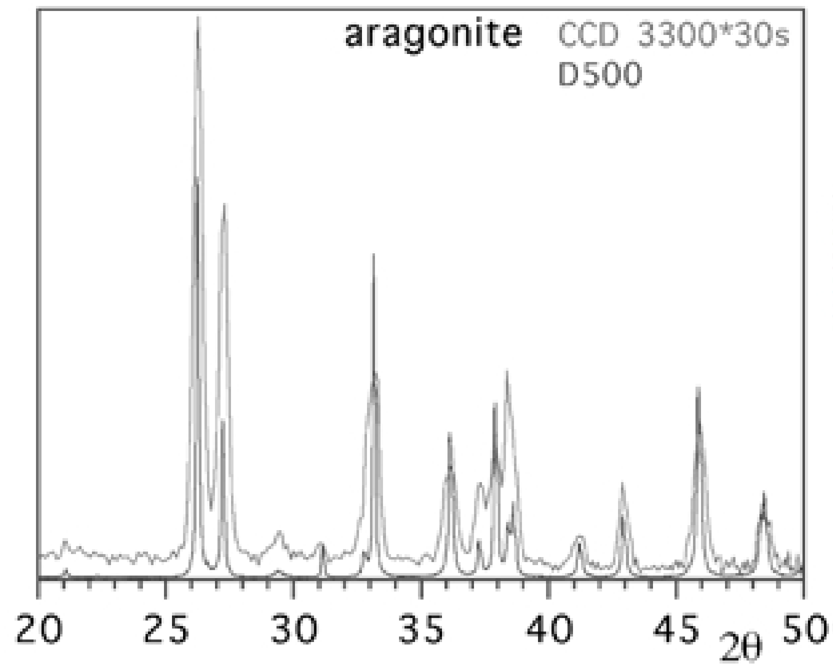

Figure 12. Aragonite diffractogram, assembled from the data of Figure 11. The inset pattern, also aragonite, was obtained using a commercial laboratory instrument. The peak width of the CHEMIN instrument is 0.2 degrees 2 theta, as compared to 0.06 degrees 2 theta for the commercial instrument. Despite the slightly greater peak width, CHEMIN data are fully quantifiable using Rietveld refinement.

X-ray fluorescence data may be obtained for elements 4<Z<92 (beryllium to uranium) (see figure 13). Energy discrimination is used to differentiate between diffracted primary beam characteristic photons and secondary fluorescence photons. The diffraction mode line resolution of 0.02 Å is sufficient to allow application of the Rietveld refinement method to the data. The proposed CHEMIN development effort will include combining diffraction and fluorescence data using simultaneous linear equations, to derive the most accurate mineral and chemical composition. A prototype version of the CHEMIN instrument, developed with NASA Planetary Instrument Definition and Development Program funding has been operable since July, 1996. ❑

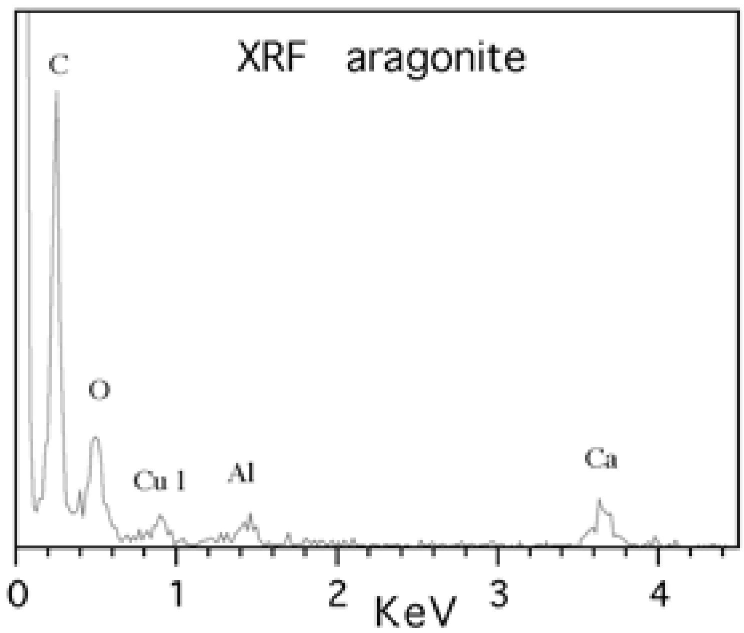

Figure 13. Aragonite XRF spectrum. Aluminum and copper X-rays originate from components of the camera system of the prototype instrument and are not part of the sample.

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Polyhydroxylated Compounds in Meteorites

George Cooper, Novelle Kimmich, and Katrina Brabham

Meteorites and interplanetary dust particles are the oldest items available for laboratory study of early solar system chemical and physical processes. Most carbonaceous meteorites, a class of meteorite relatively enriched in carbon and organic compounds, are as old or older than the solar system planets, approximately four and a half-billion years. As a group they are also the most unaltered early solar system objects as illustrated by their near solar (Sun) abundances in all but the most volatile elements. For this reason their content of organic compounds is a record of the earliest known abiotic organic synthesis. Meteorites, along with comets and interplanetary dust particles, may have delivered much organic matter to the early Earth.

The best characterized carbonaceous meteorite with respect to organic chemistry, the Murchison meteorite, has been found to contain a large number of water-soluble organic compounds. These include amino acids, carboxylic acids, dicarboxylic acids, hydroxycarboxylic acids, amides, purines, pyrimidines, phosphonates, and sulfonates. Absent among the biologically important compounds reported in meteorites are sugars, polyhydroxylated aldehydes or ketones (polyols). Ribose and deoxyribose, five carbon sugars, are central to the role of contemporary nucleic acids, DNA and RNA. If polyhydroxylated compounds are found in meteorites, this would demonstrate that such compounds could have been part of the initial mixture of prebiotic and biologically important compounds on the early Earth. If polyols, or any series of organic compounds are true products of abiotic chemistry, it seems likely that their synthesis would begin with smaller members of the series and gradually build, in decreasing abundance, to more complex members. This is the case with all homologous series of indigenous organic compounds seen in the Murchison meteorite, i.e., amino acids, carboxylic acids, amides, etc. In the case of sugars and other polyols, one of the most generally agreed upon scenarios for natural abiotic synthesis is the 'Formose' reaction. In this reaction, formaldehyde (CH_2O) in aqueous solution reacts with itself to gradually build a variety of hydroxylated compounds and sugars of increasing carbon number. Among the known products are glycoaldehyde, ethylene glycol, glyceraldehyde, dihydroxyacetone, glycerol, erythrose, ribose, six carbon sugars, etc. Because there was aqueous alteration on the parent bodies of carbonaceous meteorites and formaldehyde is a ubiquitous interstellar compound, the Formose reaction would have been possible in meteorites. Efforts at Ames have been directed towards determining the nature and abundance of polyols in carbonaceous meteorites.

The methods used for the study include isolating the meteorite polyols by ion exchange chromatography, identification by gas chromatography-mass spectrometry (GC-MS) and isotopic analysis to ensure that identified compounds are extraterrestrial and not Earthly contaminants. Preliminary analysis of Murchison extracts indicates an abiotic synthesis of polyols, i.e., a series of compounds of increasing carbon number (and decreasing abundance) have been observed. Some of the identified compounds are ethylene glycol, glycerol, dihydroxyacetone and glyceric acid. There is also evidence of higher polyols. Bulk carbon ($^{13}C/^{12}C$) and hydrogen (D/H) isotopic measurements also indicate that the majority of these compounds are indigenous to the meteorite. Determination of the isotopic composition (D/H, $^{13}C/^{12}C$, and $^{16}O/^{17}O/^{18}O$) of individual compounds as well as further bulk measurements will help to determine their synthetic origins. ❑

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Evolutionary Ecology of Microbial Communities in Yellowstone

Ken Cullings

Ecosystem function and responses of ecosystems to both human-induced and natural change are mediated to a large extent by microbial processes. While this fact is widely acknowledged, the role that different microbes play in this mediation is poorly understood. This is because the microbial community can be likened to a 'black box,' it is extremely difficult to identify microbes in their natural habitat because there are few if any physical characteristics that can be used to distinguish among them. In this research, molecular-genetic tools are being developed for microbe identification in soil samples. These tools are being used to answer fundamental questions regarding ecosystem function and microbial evolution.

One set of projects is aimed at asking to what degree co-evolution has given rise to specific interactions in a special type of plant/microbe interaction, the mycorrhizal symbiosis. Mycorrhizae are composed of plant and fungal components, and are responsible for mediating photosynthesis, carbon cycling, soil litter breakdown, and nitrogen cycling in all terrestrial ecosystems. If patterns of specificity exists in nature, and if given plant species therefore require a certain subset of fungal species to survive, then the presence or absence of given fungal species would affect ecosystem dynamics. In addition, the question of whether or not human-induced disturbance to ecosystems, such as clear-cutting, and natural disturbance, such as fire, affect mycorrhizal communities differently is being addressed.

Finally, because mycorrhizae enable plants to establish and survive in extreme environments, how mycorrhizal communities in undisturbed ecosystems and thermally-altered soils differ, and what adaptations these microbes have evolved in order to survive in these harsh environments, are being determined.

This research is taking place in the forest and hot spring ecosystems of Yellowstone Park, and is directly addressing many of these questions in the context of the 1988 fires. Results of the co-evolution experiments indicate that specific patterns of interaction have evolved between plant and fungal partners. This indicates that exclusive patterns of carbon and nitrogen flow exist in this forest ecosystem, and suggest that mycorrhizal interactions play important roles in controlling ecosystem dynamics. Furthermore, plants that arrive in the ecosystem relatively late prefer fungal species that break down the needles of the plants that precede them. Therefore, there is evidence that fungal species facilitate the establishment of new tree species, providing rare support for a facilitation model of ecosystem dynamics. This research is being expanded to determine effects of alteration of carbon flow to the roots and of litter manipulation on specificity patterns.

A parallel project addresses the hypothesis that natural burn and clear-cutting will have different effects on the mycorrhizal community. The dogma is that they will not. However there are obvious differences between fire and clear-cutting including super-heating of soils and removal of litter, an important substrate for fungi and the main source of nitrogen for trees. Initial experiments indicate that there are differences between fire and clear-cutting in the short term. Experiments are now being planned to determine whether or not these differences extend into relatively long time scales, and therefore whether or not human-induced disturbances will have long-term effects on ecosystem dynamics.

Finally, a new project has been started to determine the effects of thermal-alteration of soils on soil microbial communities. This work has direct application to Astrobiology and Exobiology in that the earliest terrestrial organisms, and possibly organisms on Mars, first evolved in hot springs environments. Migration into the surrounding soils would have followed shortly thereafter, and indeed these communities may have persisted long after thermal features dried and springs disappeared. Thus these soils are suitable models in the search for life on Mars and other terrestrial planets. Initial results indicate that acid-sulfate thermal soils are inhabited by fungi that have adapted to extremely acidic conditions, but are different from those traditionally thought to inhabit extreme acid soils. This has important implications for soil remediation strategies, and indicate that the dominant paradigm for fungal adaptation to extreme environments needs modification. This study is being expanded to include other soil microbes such as bacteria, Archea, and cyanobacteria. ❏

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Peroxy in Rocks - A Paradox

Friedemann Freund and Andrew G. Tenn

The Earth – like any other solar system body, small and large – is chemically reduced. As a result, all igneous rocks from deep within the Earth are reduced. It may therefore come as a surprise to learn that such rocks are suspected to contain peroxy, the epitome of oxidizing compounds. An experimental verification would be quite important and may affect our thinking about rocks, about some of their key geophysical and geochemical properties, and even about some puzzling observations from the realm of biology regarding the earliest life forms on Earth.

A peroxy consists of two oxygen anions. Normally, these oxygen anions carry two extra electrons to complete their outer shell and achieve a stable configuration of eight. In the case of peroxy, both oxygens have given away one of their extra electrons, leaving seven; this is not a stable configuration. By pairing up and forming a short bond of shared electrons, the peroxy is stabilized.

To 'see' peroxy in a mineral structure we have to break the oxygen–oxygen bond. When this happens, the peroxy awakens from its dormant, electrically inactive state releasing defect electrons or 'holes.' These are charges not dissimilar to the holes in a p-type semiconductor used for building transistors. As soon as the holes appear, they crowd to the surface of the molecule, leading to a positive surface charge and to an enhanced surface conductivity.

This led to a benchmark experiment. Two thin strips of gold were deposited on the surface of a single crystal of magnesium oxide to measure the surface conductivity. Figure 14 shows in (a) a view down onto the crystal on which the two thin gold electrodes, and in (b) a cross section of the conductivity cell with the crystal between two planar electrodes for applying a cross field. The breaking of peroxy bonds inside the crystal leads to an increase in the surface current because the holes come to the surface from within. We then apply a strong cross field and alternate the field direction.

Figure 15 shows how the surface current (bold solid line) changes with the application of ±1250 Volt-per-centimeter cross fields (thin dashed line). When the cross field is positive, meaning that the upper electrode in figure 14 is positively biased, the surface conductivity decreases. When the cross field is negative, the surface conductivity increases. The effect is reversible during repetitive heating and cooling cycles. Such a response is only possible if the surface conductivity is caused by charges coming to the surface from inside the crystal. The only source for such charges are the peroxy in structure.

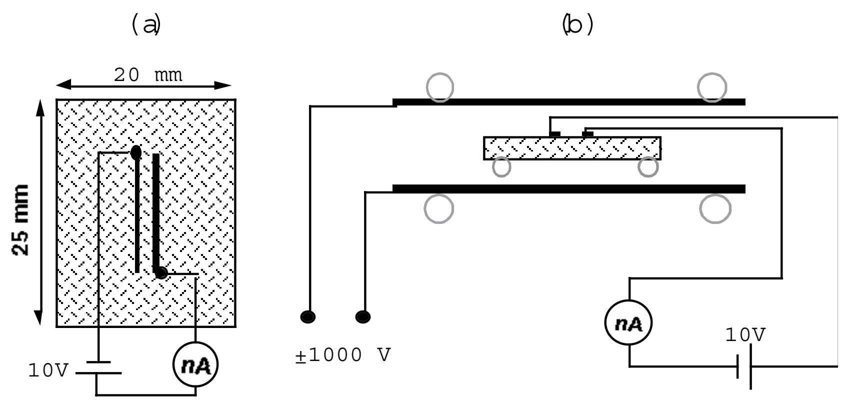

Figure 14. (a) Gold electrodes, 1 x 15 mm, 3 mm apart, sputtered onto one side of a magnesium oxide crystal (patterned) for surface current measurements; (b) Cross section of the conductivity cell with the crystal mounted between two electrodes for application of ±1250 V/cm cross fields.

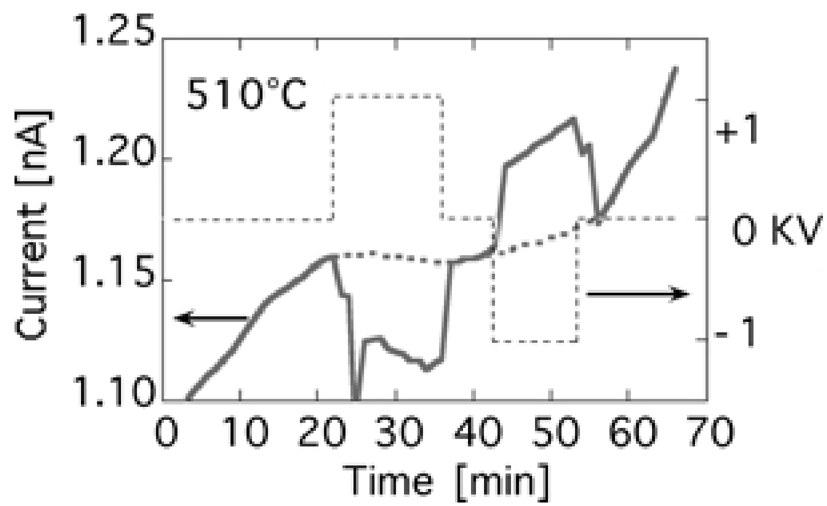

Figure 15. Upon application of +1000 V cross voltage the surface current decreases while at a cross voltage of –1000 V it increases. This is proof positive that the current is carried by positive charges, so-called holes, and that these charges exist inside the magnesium oxide crystal. The baseline drift is caused by slight temperature variations during the run.

Next the surface of the crystal was covered with a very thin layer of carbon and its conductivity re-measured. The conductivity was uniformly higher, indicating that it was dominated by current flowing through the thin carbon film. Application of the ±1250 V cross fields now ceased to have any effect on the surface current because the electrons flowing through the film are completely separate from the charges that move to and fro inside the crystal.

This experiment provides proof positive that peroxy exist in a crystal like this magnesium oxide which had been grown from a highly reduced melt and should therefore never contain anything as oxidized as peroxy. The reason why peroxy got into the crystal has to do with the small amount of water that became incorporated when the magnesium oxide crystallized from the melt. During cooling, this dissolved water converted to peroxy and hydrogen. With knowledge available from other studies it is possible to boldly extrapolate to rocks. All igneous rocks on Earth and Mars have solidified from magmas, generally highly reduced and always saturated with water. Based on these experiments, the minerals in these rocks should therefore contain peroxy.

The presence of peroxy has implications for many geophysical questions related to the electrical conductivity of the Earth's deeper crust and to phenomena associated with earthquakes. Another aspect relates to the earliest life forms on Earth. Rocks that contain peroxy, when they weather, will release hydrogen peroxide. Any early organism living on such a rock surface will therefore experience a constant trickle of hydrogen peroxide, a potentially lethal oxidant. Assuming that early organisms lived in close contact with rocks and secreted acids which etched the rock surface away, these organisms were forced to develop a defense mechanism against this powerful oxidant. It has long puzzled observers that antioxidant enzymes appear deeply rooted on the tree of Life, implying that these enzymes were 'invented' early in life's evolution, long before there was free oxygen gas in the Earth's atmosphere. Peroxy in the rocks and hydrogen peroxide at the rock-water interface may have been the driving force behind this important early evolutionary step. ❑

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2-Methylhopanids: Biomarkers for Ancient Cyanobacterial Communities

Linda L. Jahnke, Roger E. Summons and Harold P. Klein

A variety of microbially mediated processes contributed to the cycling of carbon in ancient microbial ecosystems. These processes can sometimes be characterized by the identification of remnant cellular compounds ('biomarker molecules') in ancient sedimentary organic matter. One of the important goals of biomarker analysis is to link these ancient chemical fossils to modern day organisms and understand through study of contemporary environments how much biomarkers are deposited, how they survive, and what they tell about the evolution of ancient microbial communities. An important new tool in this work is being applied to biomarker analysis. Compound specific isotope analysis (CSIA) allows measurement of the relative amounts of carbon-12 (^{12}C) and carbon-13 (^{13}C) in any compound which can be chromatographically separated using a gas chromatograph-combustion-isotope ratio mass spectrometer (GC-C-IRMS). Biochemical processes often result in the synthesis of molecules depleted in ^{13}C relative to ^{12}C. Such carbon isotopic fractionations are described by the term 'delta C13' ($\partial^{13}C$). CSIA allows us to determine $\partial^{13}C$ values for individual organic compounds. This is important because as carbon is cycled through a microbial community the preference of biological systems for ^{12}C leads to synthesis of lighter biomarker molecules as the carbon flow approaches terminal processes, so that an additional degree of taxonomic attribution results in measurement of the ∂13C.

Life began on the early Earth in an environment devoid of free molecular oxygen (O_2) in the atmosphere. The rise of O_2 in the atmosphere, as a consequence of the evolution of oxygenic photosynthesis, had a profound effect on the subsequent progression of the Earth's biological evolution and geological history. Oxygenic photosynthesis evolved within the cyanobacterial lineage, however, evidence for the timing of this event remains obscured within the molecular and rock records. By studying the molecular structure and carbon isotopic composition of lipid biomarkers in cyanobacteria, we seek to link modern day cyanobacteria and their microbial mat analog environments to an ancient organic record.

The bacteriohopanepolyols (BHP) are a group of amphiphilic membrane biochemicals which are a particularly important group of biomarker molecules because the hydrocarbon skeletons of BHP are extremely refractory and survive sedimentary diagenesis. The geohopanes may well be the most abundant class of natural products on the Earth. BHP are widespread among the aerobic bacteria and

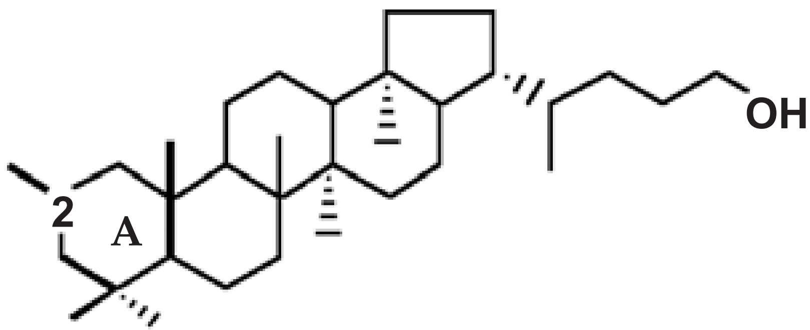

Figure 16. 2-Methylbacteriohopanol is one example of a class of amphiphilic membrane biochemicals which are a particularly important group of biomarker molecules.

therefore, only of general taxonomic use. A supplementary methyl substituent at the 2-position of ring-A of the pentacyclic triterpane skeleton, however, may provide some degree of biomarker specificity (see Figure 16).

Similar 2-methyhopanes have been identified in 2.5 billion year old organic rich shales by a member of our group (R.E. Summons, Australia Geological Survey Organization). Our culture studies of a taxonomically diverse spectrum of cyanobacteria has shown that methylation at C-2 is common. We have found that 2-methylbacteriohopanols (2-Me-BHP) are prominent membrane lipids in approximately 43% of cultured cyanobacteria and a number of cyanobacteria-dominated environmental mat samples. Although not exclusive to this group of bacteria, the only other known sources of 2-Me-BHP occupy specialist environmental niches and do not appear capable of providing any quantitatively important contribution to sediments. 2-Me-BHP carry a readily measured molecular ^{13}C signature that will extend their usefulness as organism-specific biomarkers. Cyanobacteria are photoautotrophs using the energy of sunlight to convert carbon dioxide to cellular components, and as discussed above, such biological processes can result in carbon isotope fractionation. We have found that the BHP synthesized as a result of cyanobacterial, photoautotrophic growth are depleted in ^{13}C by 28 per mil relative to the carbon dioxide source with the 2-Me-BHP about 2 per mil heavier than its non-methylated analog. Similar carbon isotopic patterns have been measured for the 2-methyl and non-methyl BHPs in natural environmental samples establishing an isotopic signature for cyanobacterial BHP. Knowledge of the fractionation factors accompanying their biosynthesis also accord the potential to use 2-Me-BHP to determine the isotopic composition of inorganic carbon in modern aquatic and marine environments and their analogues in the fossil record. ❑

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Simulations of a Model Transmembrane Proton Transport System

Karl Schweighofer and Andrew Pohorille

The transport of protons across membranes is an essential process for both bioenergetics of modern cells and the origins of cellular life. All living systems make use of proton gradients across cell walls to convert environmental energy into a high-energy chemical compound, adenosine triphosphate (ATP). ATP, in turn, is used as a source of energy to drive many cellular reactions. The ubiquity of this process in biology suggests that even the earliest cellular systems were relying on proton gradient for harvesting environmental energy needed to support their survival and growth. In contemporary cells, proton transfer is assisted by large, complex proteins embedded in membranes. The issue addressed in this study was: how the same process can be accomplished with the aid of similar, but much simpler molecules that could have existed in the protobiological milieu?

The model system used in the study contained a bilayer membrane made of phospholipid, dimyristoylphosphatidylcholine (DMPC), which is a good model of the biological membranes forming cellular boundaries. Both sides of the bilayer were surrounded by water that simulated the environment inside and outside the cell. Embedded in the membrane was a fragment of the Influenza-A M_2 protein, and enough sodium counter ions to maintain system neutrality (see Figure 17).

This protein has been shown to exhibit remarkably high rates of proton transport and, therefore, is an excellent model to study the formation of proton gradients across membranes. The Influenza M_2 protein is 97 amino acids in length, but a fragment 25 amino acids long, which contains a transmembrane domain of 19 amino acids flanked by 3 amino acids on each side, is sufficient to transport protons. Four identical protein fragments, each folded into a helix, aggregate to form small channels spanning the membrane. Protons are conducted through a narrow pore in the middle of the channel, in response to an applied voltage. This channel is large enough to contain water molecules, and is normally filled with water.

In analogy to the mechanism of proton transfer in some other channels, it has been postulated that protons are translocated along the network of water molecules filling the pore of the channel. This mechanism, however, must involve an additional, important step because the channel contains four histidine amino acid residues, one from each of the helices, which are sufficiently large to occlude the pore and interrupt the water network. The histidine residues ensure channel selectivity by blocking transport of small ions, such as sodium or potassium. They have been also implicated in gating protons due to the ability of each histidine to become positively charged by accepting an additional proton. Two mechanisms of gating have been proposed.

In one mechanism, all four histidines acquire an additional proton and, due to repulsion between their positive charges, move away from one another, thus opening the channel. The alternative mechanism relies on the ability of protons to move between different atoms in a molecule (tautomerization). Thus, a proton is captured on one side of the gate while another proton is released from the opposite side, and the molecule returns to the initial state through tautomerization. The simulations were designed to test these two mechanisms.

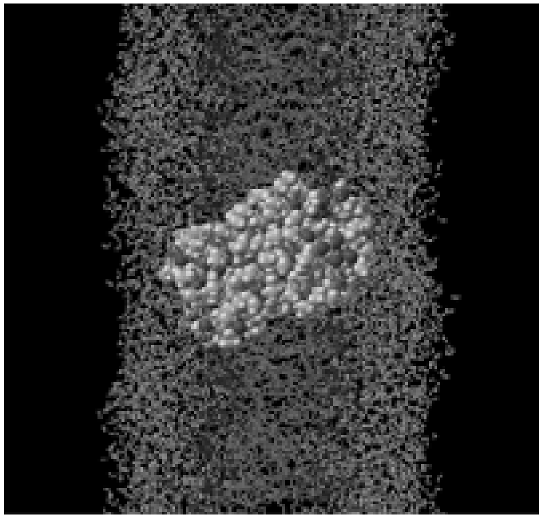

Figure 17. This figure shows the M_2 protein embedded in a DMPC membrane which is flanked by water layers. Both the water, and the membrane are represented by sticks, whereas the protein is rendered as spherical or 'cpk.' The color legend is as follows: water hydrogen (cyan), water oxygen (magenta), membrane hydrocarbon tails (green), membrane head groups (blue), sodium ions (yellow cpk), protein (multicolored cpk). The protein is clearly tilted in the bilayer, which helps it maintain favorable interactions with the interior of the membrane. Water in the channel cannot be seen because of the opacity of the protein in this figure.

Large-scale, atomic-level molecular dynamics simulations of the channel, with the histidine residues in different protonation states, revealed that all intermediate states of the system involved in the tautomerization mechanism are structurally stable and the arrangement of water molecules in the channel is conducive to the proton transport. In contrast, in the four-protonated state, postulated to exist in the gate-opening mechanism, the electrostatic repulsion between the histidine residues appears to be so large that the channel looses its structural integrity and one helix moves away from the remaining three. This result indicates that such a mechanism of proton transport is unlikely.

The simulations revealed that translocation along a network of water molecules in the channel and tautomerization of the histidine residues in the M_2 proteins is the most likely mechanism of proton transport. The results not only explain how a remarkably simple protein system can efficiently aid in the formation of proton gradients across cell walls, but also suggest how this system can be genetically re-engineered to become a directional, reversible proton pump. Such a pump can provide energy to laboratory-built models of simple cellular systems. If they were successfully constructed, it would greatly advance our understanding of the beginnings of life and find important applications in medicine and pharmacology. ❏

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Molecular Imprinting of Polymeric Columns

Thomas Shen, Jay Chen, and Narcinda Lerner

L-amino acids are one of the fundamental building blocks of living organisms. Because of this, their detection at trace levels is one of the major targets of many programs searching for the origin of life. L-amino acids have an advantage over other biomarkers in that they contain a chiral center, which is considered as a 'biosignature' for the presence of life. Amino acids of abiotic origin are racemic, with equal amounts of the L-form and the D-form. Any biological debris remaining from chemical and/or biological evolution on Mars or other planetary bodies would be present in trace amounts due to decay over millions or billions of years. Highly sensitive instruments will be required to detect such debris in situ as well as in measurements of returned samples from planetary flight missions.

Molecular imprinting is a simple and convenient way to prepare antibody-like materials which have been increasingly used in separation science and, more recently, sensing technology. The principle of this technique, including surface attachment and in situ polymerization, is described in Figure 18. Using this technology, very small amount of amino acids or biomolecules can be concentrated and separated for detection.

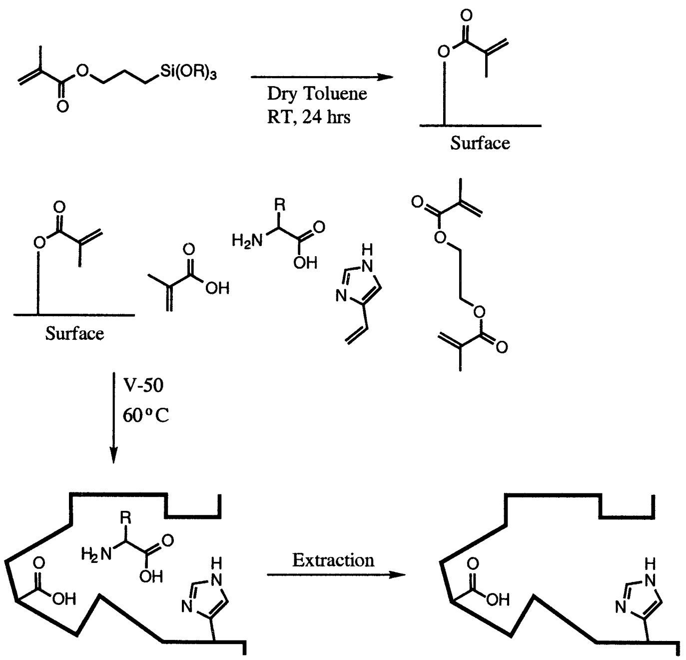

Figure 18. The preparation of surface-linked molecular imprinting polymeric columns.

Recently, the reaction conditions for preparing molecularly imprinted polymers (MIP) for amino acid separation were developed. The results indicated that the template effect exists by comparison of the binding effects between molecularly imprinted polymers and the control polymers. Approximately up to 1 microgram (µg) of L-phenylalanine (L-phe) could be absorbed by 1 milligram (mg) of L-phenylalanine-imprinted polymers.

Experiments on coating a capillary column with the L-phe-imprinted polymer by in situ polymerization were also studied. The inner surface of the capillary was first coated with a layer of the monomer trimethoxysilylpropyl methacrylate and then in situ polymerization was conducted inside the column (inner diameter = 0.53 millimeter) in the presence of L-phe.

Visual observation indicates that the capillary coated with the L-phe-imprinted polymer displays a nice layer of MIP coating on the inner surface of the column. The bonded polymer layer could be observed readily without instrumentation. Further analysis based on scanning microscopy will provide information regarding the bonding structure of this coating. The good structural stability of the stationary phase produced by this procedure will allow its use in the production of capillaries with reduced inner diameter i.e. micro-columns on glass chips. The success of coating the micro-columns with the MIPs will make possible miniaturized capillary electro-chroamtography with a stationary phase designed specifically for targeted molecules.

Preliminary results indicate that small amounts of non-specific absorption also occurred, therefore, further improvement is in progress. ❑

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Prebiotic Synthesis of Activated Amino Acids

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Chemical processes occurring on the primitive Earth about four billion years ago yielded molecules that had the ability to make copies of themselves (replicate). These rudimentary replicating molecules eventually developed into today's life that uses both protein and DNA molecules for replication. Since the DNA used by modern biota is too complex to have been chemically made on the primitive Earth, the first replicating systems may have been composed solely of small proteins ('peptides'). Peptides are good candidates for the first replicating molecules because they are constructed from very simple building blocks – activated amino acid molecules – which could have been made by chemical processes on the primitive Earth.

To determine how activated amino acid and peptide molecules could have been generated on, or delivered to the primitive Earth four billion years ago three distinct research areas were pursued: 1) the catalysis of sugar synthesis and its conversion to activated amino acids was investigated in the laboratory under simulated primitive Earth conditions, 2) the energy of carbon-carbon bond formation and cleavage for different carbon groups was calculated to evaluate the constraining role of thermodynamics in prebiotic carbon chemistry leading to the origin of life and metabolism, and 3) samples of the Cretaceous-Tertiary boundary layer were analyzed for extraterrestrial amino acids to see if they survived the meteorite impact that delivered them to Earth. In the past year significant progress was made in these three research areas.

Amines (including amino acids) were shown to catalyze the prebiotic pathway (discovered last year) that generates activated amino acid thioesters capable of forming peptides. Specifically, amines were found to catalyze the first two reactions of the prebiotic pathway (aldol condensation and dehydration) involved in the synthesis of alanine and homoserine thioesters from formaldehyde and glycolaldehyde. Catalysis of the first two steps of this pathway by alanine, itself a product of the pathway, demonstrates that this prebiotic pathway has the potential to function autocatalytically. This pathway is an attractive prebiotic process because it operates under mild aqueous conditions, and like modern amino acid biosynthesis, uses sugar intermediates which are converted to amino acids by energy-yielding redox reactions.

The second line of investigation was to identify the thermodynamic constraints that govern carbon chemistry involved in the origin of life. The free energy was calculated for the formation and cleavage of 100 carbon-carbon bond combinations made from 10 different aliphatic carbon groups. Overall, this analysis showed that thermodynamics acts to constrain the carbon chemistry of the origin of life to reactions that proceed by redox disproportionation. In disproportionation in which the more oxidized carbon group of a reacting pair of carbons becomes more oxidized, and the more reduced carbon group of the pair becomes more reduced. Furthermore, the analysis revealed three interesting characteristics of carbon bonds: a) carbon bonds to carbonyl groups are very unstable, making them easy to cleave but hard to make, b) alcohol groups are moderately unstable, making them more difficult to cleave but not hard to make, and c) hydrocarbon groups are very stable, making them very difficult to cleave but not hard to make.

In the final area of investigation, and in preparation for the analysis of the martian meteorite ALH84001, samples of Cretaceous-Tertiary boundary sediments were analyzed for extraterrestrial amino acids. A sample of Cretaceous-Tertiary boundary sediment from Sussex Wyoming was shown to contain about 310 picomoles per gram of the meteoritic amino acid, α-amino-isobutyric acid. Knowledge of the amino acids in extraterrestrial materials, such as meteorites, contributes to understanding the processes involved in the delivery of amino acids to the primitive Earth during the origin of life. ❑

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Astrobiology Technology Branch Overview

The Astrobiology Technology Branch supports the development of advanced technologies in astrobiology as they relate to the exploration of space and understanding life in the universe. Current branch efforts encompass research and technology development for advanced life support, utilization of planetary resources, astrobiology advanced missions, and technology transfer to benefit life on Earth. Advanced Life Support focused research is directed primarily at physicochemical processes for use in regenerative life support systems required for future human missions and includes atmosphere revitalization, water recovery, waste processing/resource recovery, and systems modeling, analysis and controls associated with integrated subsystems operation. *In Situ* Resource Utilization (ISRU) technologies will become increasingly important on every Mars lander between 2001 and a human mission to Mars. The branch focus is on the development of technologies for Mars atmosphere acquisition, buffer gas production, and CO_2 compression. Research and technology development for astrobiology advanced missions includes the development of technologies for hydrothermal vent "missions," piggyback Europa penetrators, artificial ecosystems, and systems for planetary ecology detection. The Multiple Sclerosis Technology Transfer program is a spin-off application of astronaut cooling garments, with research focused on utilization of this technology by heat sensitive Multiple Sclerosis patients to alleviate symptoms and improve quality of life. Researchers in the branch also develop flight experiments and associated hardware for shuttle, ISS, and unmanned NASA missions.

M. Kliss, Chief SSR

Advanced Life Support Research and Technology Development

Mark Kliss

The research and development of advanced life support technologies at Ames Research Center will help enable long duration missions and the human exploration and development of space. The major objectives of advanced life support research is to: 1) reduce life support system life cycle costs, 2) improve operational performance, 3) promote self-sufficiency, and 4) minimize expenditure of resources during long duration human missions. The main focus of the research at Ames in 1998 was on waste processing and resource recovery, modeling and analysis, and In Situ Resource Utilization (ISRU).

Waste processing systems that eliminate noxious wastes are a necessary component of any fully regenerative life support system that incorporates food production. Waste processing can be accomplished by either biological or physical-chemical systems. The optimum method of processing is dependent on the ability of food production systems and humans to reutilize the reclaimed materials. A thorough understanding of the impurities in the reclaimed materials and the effect of these impurities on plants and humans is required in the development of waste processing systems. The research effort was focused on integrating a prototype incinerator, developed by Ames Research Center, with a catalytic test stand in order to evaluate newly developed catalyst systems. Of primary interest was the use of an advanced catalyst to remove nitrogen dioxide and nitric oxide from the incinerator flue gas by reducing them with carbon monoxide to form nitrogen and oxygen. This approach is extremely promising because it requires no additional chemicals, such as ammonia, for the reduction process. Using carbon monoxide at concentrations of several thousand parts per million, it was demonstrated that nitrogen oxides can be reduced in incinerator flue gas from concentrations of 50 parts per million to less than 1 part per million.

For the modeling and analysis research effort at Ames, data from existing literature, universities, and other NASA Centers was utilized to develop individual crop models for the candidate crops that might be incorporated into the ‘BIO-Plex’ human-rated advanced life support test chamber at Johnson Space Center. The models accounted for carbon dioxide uptake, oxygen production, edible and inedible biomass production, water vapor production, and water uptake from the nutrient solution as functions of the carbon dioxide concentration, light level, and crop growth area. The models were then used to evaluate system management and operations issues and to conduct system trade studies. It was shown in a comparison of separate (multiple) and single air loop configurations that as long as food production rates are greater than 50% of crew requirements, the existing air revitalization system can be eliminated and a single loop air revitalization system linking the crew chambers, food production chambers and waste processing systems can adequately control the carbon dioxide level by varying the solid waste processing rate. Scientific analyses of soil and rock samples on Mars will require the use of carrier gases such as nitrogen and argon for moving analytes and purging instrumentation. The ISRU research efforts at Ames relating to the 'mining' of Mars' atmosphere, culminated in the development of demonstration hardware which is capable of separating and purifying a nitrogen-argon carrier gas mixture away from the martian atmosphere and compressing the mixture to a usable pressure. Both the separation and compression processes were performed via adsorption. In addition to being low-mass, low-volume, and virtually solid state, the process consumes virtually no electrical power since the energy to perform work is taken entirely from the Mars diurnal temperature cycle. Figure 19 shows a concept drawing of such a device. It weighs less than 100 grams, occupies a volume roughly equal to a 12-ounce soda can, and produces enough carrier gas for several analyses a week for an indefinite period of time. This technology is applicable to all lander and rover missions to Mars and has other possible uses both within NASA, by providing compressed carbon dioxide for generating buffer gases for life support, and in the private sector, by producing purified compressed gases in remote locations or in applications having stringent restrictions on power, noise, or vibration. ❑

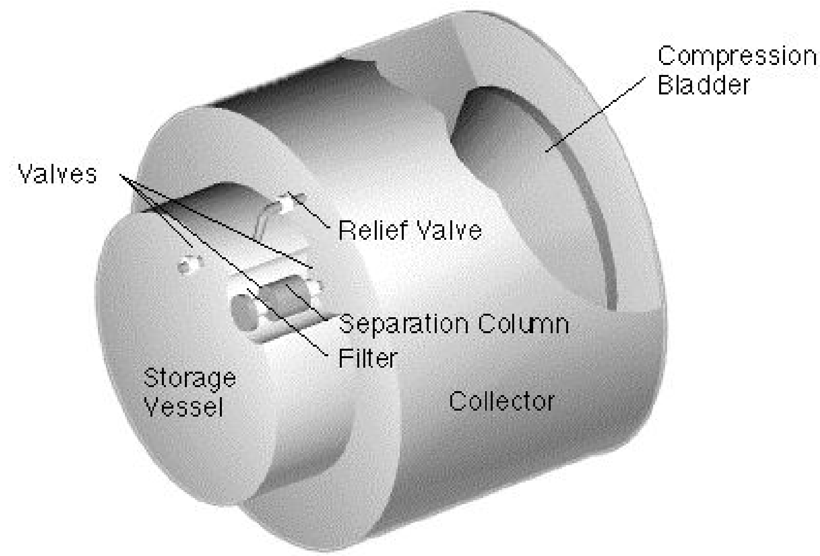

Figure 19. A concept drawing of ISRU hardware which can extract and compress carrier gases from the martian atmosphere.

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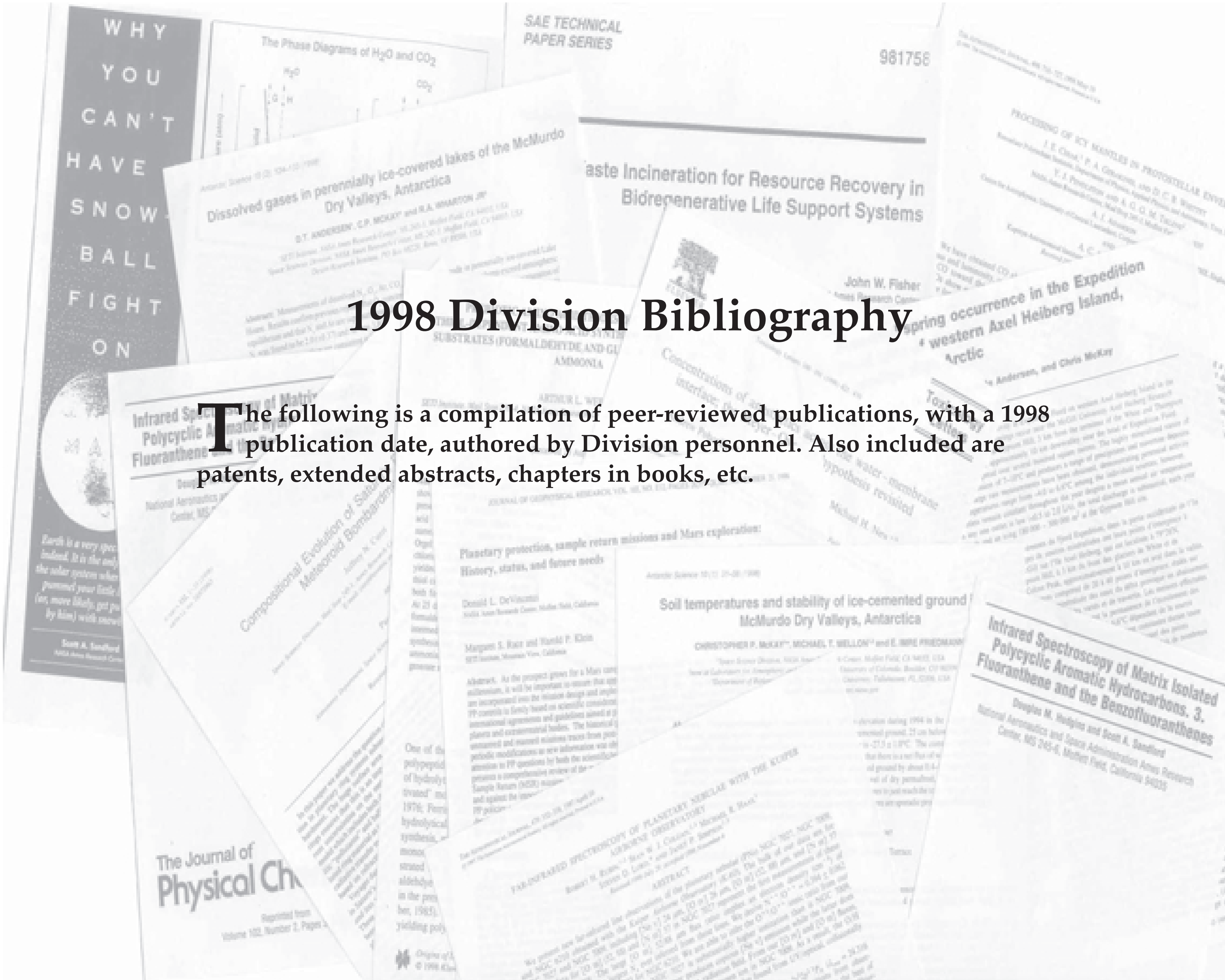

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