
University of Arizona

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An Astronomical Search for the Essential Ingredients for Life: Placing our Habitable System in Context

Principal Investigator:

Neville Woolf nwoolf@as.arizona.edu

Co-Investigators/Collaborators:

At University of Arizona:

Ludwik Adamowicz	Renu Malhotra
J. Roger Angel	Michael Meyer
Aldo Apponi	Robin Polt
Michael Brown	Edward Prather
Adam Burrows	Timothy Slater
Laird Close	Peter Strittmatter
Philip Hinz	Christopher Walker
David Kring	Lucy Ziurys
Jonathan Lunine	

Mark Giampapa, *National Solar Observatory*
Alfred Glassgold, *University of California, Berkeley*
Eric Herbst, *The Ohio State University*
Joan Najita, *NOAO*
Stephen Strom, *NOAO*

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Executive Summary

We plan to carry out three investigations concerning the astronomical constraints on the possible origins of life in the Universe.

Our first module will focus on astrochemical investigations concerning the building blocks of life. Under the leadership of L. Ziurys, we plan to: (i) undertake laboratory studies to determine signatures for pre-biotic compounds that might exist in the interstellar medium, with special emphasis on ribose; (ii) initiate an observational search for these gas-phase molecules that are important for life using millimeter and sub-millimeter radio telescopes to which we have access; and (iii) conduct theoretical studies into the stability of complex organic molecules in the gas phase ISM and the evolution of their abundances in circumstellar disks in order to interpret the broader implications of our findings for the possibility of life elsewhere in the Universe. This module will address Goal #3 in the NAI revised roadmap.

Our second module will focus on the formation and evolution of habitable worlds under the leadership of S. Strom and J. Najita (NOAO). We plan to: (i) undertake an observational program to learn when, where, and how frequently planets form around young stars to provide the possibility for constraints on habitable planet formation; (ii) conduct an observational characterization of circumstellar environments that give rise to life and initiate a theoretical modeling program to determine the frequency of giant impacts as traced through circumstellar dust disk evolution, connecting the evolution of dusty disks around sunlike stars to the history of our solar system; and (iii) investigate the time evolution of the UV/x-ray flux of young solar-type stars from the protostellar phase through the epoch of terrestrial planet formation to mature planetary systems. The investigation will also include studies of stars that have evolved further than the Sun, so as to predict the future variability of the Sun. This module addresses Goal #1 of the NAI Revised Roadmap, as well as aspects of #4 and #6.

Our third module, under the leadership of R. Angel and P. Hinz and is aimed at the characterization of planetary systems. We plan to: (i) initiate an observational program aimed at the direct detection and characterization of astrobiochemically relevant extra-solar giant planets (EGPs) to determine their frequency around solar-type stars and characterize their composition through spectroscopy; (ii) initiate a theoretical study of giant planet atmospheres extending current modeling efforts down to $0.1 M_{\text{Jupiter}}$ as a first step in understanding the detectability of biosignatures in planet atmospheres with liquid water present; and (iii) extend observational work on the observed earthshine spectrum to near-infrared wavelengths to close a gap in our understanding as well as initiate a monitoring program. This module addresses goals #1 and #7 in the NAI Revised Roadmap.

Our special emphasis on the revised roadmap Goal #1 arises because of current lack of understanding of how the Solar System arose, and how it fits with the many other planetary systems which are being discovered, and which have substantial differences from the Solar System. Our goal is to set a better, more appropriate starting point for consideration of the origin of life, and to start to explore the question of whether Earth is or is not rare.

Our plans to strengthen the astrobiology community revolve around the creation of the Laplace Center for interdisciplinary astrobiology studies and the Astrobiology Winter School to be held annually here at the University of Arizona. The Laplace Center will be an interdisciplinary program (IDP), a standard system for interdisciplinary research and teaching at UA. It will serve as a focus for our interdisciplinary research efforts and strengthen the growing ties between the Departments of Astronomy, Planetary Sciences, NOAO, Geosciences, Chemistry and Biochemistry. Future plans call for including also Microbiology

and Ecology and Evolutionary Biology as well as the Tree Ring Laboratory, Optical Sciences, and parts of the Medical College.

The Center will host 2-3 extended visitors per year and organize meetings to increase scientific interactions across the boundaries that exist within the College of Science. The Winter School will train up to twenty students per year over the period of performance of this proposal. We plan to host visiting faculty for up to two months per year from partner NAI node institutions as well as 10 graduate students for a four-month curriculum in the origins of life. In collaboration with colleagues throughout the College of Science we will offer two interdisciplinary courses for graduate credit that focus on the boundaries between the disciplines and take advantage of the unique observational and laboratory facilities on the University of Arizona campus.

Our efforts to “Strengthen the Astrobiology Community” will include production of first rate scholars in areas important to the future success of the field. In addition to extant interdisciplinary graduate programs at the University of Arizona such as those in Planetary Science (Astrobiology Minor), Chemistry (Astrochemistry emphasis), and Optical Sciences (various joint degree programs) we will introduce an Astrobiology minor as part of the IDP for the departments within the College of Science.

A particularly innovative part of this proposed project is for a significant and integrated education and public outreach component led by Tim Slater. Because a comprehensive program to improve the public’s understanding of the this interdisciplinary science requires targeting schools, we will work directly with secondary school teachers on improving their understanding of the myriad of underlying concepts surrounding the search for other worlds. Initially, we plan to conduct systematic studies of the understanding and beliefs about the scientific search for other worlds held by K-14 students, teachers, and the general public. In addition to contributing to the scholarly literature base of science education, a detailed understanding of the existing notions and attitudes people have about this interdisciplinary science are crucial to designing the most effective education and public outreach programs. This will be accomplished through a systematic series of surveys, interviews, and carefully monitored instructional interventions. The results will be disseminated through journal articles and presentations at professional education conferences.

Finally, we also plan to help other graduate students and university faculty supported by this program to become informed about the reasoning difficulties K-12 students, teachers, and the general public have with understanding the search for other worlds. If research scientists have an appreciation for the specific parts of this science that people find difficult, they will be better able to communicate the exciting results and enhance the public's attitudes toward supporting this endeavor. This will be accomplished by conducting frequent workshops and contributing scholarly papers at professional science conferences as well as regularly contributing to the program's seminar series. In support of these efforts, the team will undertake the creation and dissemination of an astrobiology public speakers toolkit and a dynamic FAQ (frequently asked questions).

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I. Introduction

I.1 Rationale for the Proposal.

The ultimate goal of astrobiology is to understand the origin of life and its prevalence in the universe. There would be no purpose for astrobiological studies if it were known that life is unique to the Earth or even to the Solar System. If it is not, astrobiology studies must include investigation of a wide range of phenomena that have traditionally been viewed as principally astronomical in nature. These include the composition and dynamics of material involved in the process of star and planet formation from its initial state in interstellar clouds to its final state in planetary systems. It is also critical to understand the nature of planetary systems, the stability of the planetary environment and the influence of this environment on the evolution of life forms.

Progress in each of these areas depends on the developing the right overall balance of astronomy, geosciences, chemistry and biology input in NASA's Astrobiology Institute (NAI) as contributed by each of its individual members. It is also important to develop a common language and understanding between the various sub-disciplines, especially among the young scientists entering the field. As noted by the National Academy Committee on Extra-Terrestrial Life (COEL), the NAI program would benefit from strengthening its astronomical aspects. In submitting this proposal, we seek to contribute to the pioneering efforts at the NAI, building on the strengths and interests of the proposing organizations, the University of Arizona (UA) and the National Optical Astronomy Observatories (NOAO), both based in Tucson, Arizona. Our goal is to bring our existing strengths together to focus on the needed astronomically oriented aspects of astrobiology and to ensure that these are well meshed with other parts of the NAI program. We believe that the search for the origin of life, and the related question of the frequency of the occurrence of life in our galaxy and the universe are potentially the most interesting and challenging topics in all of 21st century science.

I.2 The Astrobiology Challenge

The current goals of NASA's Astrobiology program and hence for the NAI have been set out in the 2002 Astrobiology Roadmap. They are, in no particular order of priority:

1. Understand the nature and distribution of habitable environments in the Universe.
2. Explore for past and present habitable environments, prebiotic chemistry and signs of life elsewhere in our Solar System.
3. Understand how life emerges from cosmic and planetary precursors
4. Understand how past life on Earth interacted with its changing planetary and Solar System environment.
5. Understand the evolutionary mechanisms and the environmental limits of life.
6. Understand the principles that will shape the future of life both on Earth and beyond.
7. Determine how to recognize signatures of life on other worlds and on early Earth.

This is indeed a challenging list of objectives and explains why the NAI is a virtual institute by necessity. It is recognized within and outside of NASA that no single academic or research institution has or can have the breadth of research disciplines to meet all the Astrobiology

Roadmap goals. In its short history thus far, it has been helpful for the NAI to get started with specialized organizations, but the progress of astrobiology requires broader range of science capabilities than is currently in the NAI mix. Thus the COEL, in its review of NASA's astrobiology program, notes:

" The "astro" in astrobiology: Astronomy remains the key fundamental discipline that has yet to fully impact the discipline of astrobiology."

and

" The research interactions between these two areas [Astronomical Origins and Astrobiology] seems much weaker at the moment than they could be, and certainly much weaker than between Astrobiology and the evolutionary biology or geobiological communities."

The goal of the present collaboration is to contribute a strong astronomical element to the NAI program and to develop connections with chemistry and biochemistry. We believe that, in this way, we can help strengthen the overall NAI program in exactly the way envisaged by COEL.

I.3 The Proposed Collaborators

This proposal represents a collaboration between the UA and NOAO. The UA is a major public university in the southwestern United States with a dual mission in research and education in fields relevant to the NAI such as astronomy, planetary sciences, chemistry, geosciences, and the biological sciences. The NOAO is a major national institution for research in astronomy located on the UA campus. Both institutions can offer access to significant research facilities, with observational capability over the wavelength range from 3mm to 0.3 microns. The UA will, through Steward Observatory, be able to support the work proposed here with access to optical/infrared telescopes such as the Large Binocular Telescope (11.8m effective aperture), the MMT (6.5m), many smaller telescopes in the Tucson area, and access to the twin Magellan 6.5m telescopes in the southern hemisphere. It will also provide access to mm-wave (12m) and submm-wave (10m) telescopes. NOAO operates observatory facilities both in Tucson and in Chile. Through the UA, the collaborators can address another COEL concern, namely the needed access to major astronomical facilities.

" Much larger optical telescopes, of mirror aperture 6 meters or larger and equipped with advanced adaptive optics capabilities, are required to examine the broader class of extra-solar planets that are not in the unusual orbital orientation necessary to make studies of transit possible. Such facilities, supported outside of NASA with other federal, private or state funds, represent a substantial monetary contribution to the field of astrobiology, on a level of hundreds of millions of dollars in infrastructure."

In addition the UA has major programs in astrochemistry, planetary sciences and optical sciences that will contribute to a Tucson node of the NAI. The science of astrobiology and the activities of an Astrobiology Institute will thrive in a university setting where cross-disciplinary interactions can occur readily.

I.4 Proposed Location

We also believe that establishing an Astrobiology node in Tucson will also bring enormous benefits to the national astrobiology program. In addition to the collaborating institutions, there are many other organizations that own or share astronomical facilities based in Tucson. These include the National Radio Astronomy Observatories, the Harvard Smithsonian Center for Astrophysics, international organizations such as the German (Max-Planck-Society) and Italian (Istituto Nacional di Astrofisica) partnership in the Large Binocular Telescope, as well as individual private and public universities. Thus Tucson is a crossroads for the international astronomical community. An astrobiology center in Tucson would have a wide reaching impact on astronomical studies as well as providing a forum for interdisciplinary research across the fields of the physical and biological sciences throughout the University of Arizona. It would also complement the more geology-oriented efforts being made at the Arizona State University under the NAI program. The Center will be housed in the Astronomy Department/Steward Observatory building on campus, in close proximity to the Planetary Sciences Department/Lunar and Planetary Lab and the NOAO headquarters building.

I.5 Proposal Overview

Our proposal consists of three research modules, which range from biochemistry to astrophysics but focused on the astronomical origin of and likely harbors for life. These three modules deal respectively with questions in astrochemistry, planet formation and evolution, and characterization of extra-solar planets. They are summarized in section I.8. Section 6 describes an education and outreach plan designed to strengthen astrobiology in the community and to develop the next (perhaps the first) generation of true astrobiologists.

If selected, we plan to create a center, the **Life And P**lanets **A**strobiology **C**enter—the **LAPLACE**—within the College of Science at the UA to support and promote interdisciplinary studies towards astrobiology. The center is named to recognize the work of 18th century mathematician, Pierre Simon de Laplace, on the origin and the stability of our solar system, in *Systeme du Monde* and *Mechanique Celeste*. He also developed ideas in probability theory that will be essential in discriminating between different concepts about the origin and development of life.

The purpose of the Laplace Center is to address the problems facing the development of the astrobiology community, namely the range of disciplines and hence language required to make progress in the field and the current unwillingness of many scientists to venture across disciplinary boundaries. It is our conviction that, in time, astronomy will become increasingly concerned with astrobiology and vice-versa. The Laplace Center will accelerate that process, providing a focus for astrobiology in Tucson that transcends departmental and institutional boundaries.

A novel and major item in our proposal is the development of a Winter Astrobiology School at the UA, where we would for one complete semester each year train 20 graduate students (10 from outside the UA) in astrobiology. We would also bring in visiting faculty to complement our local expertise, especially in areas such as molecular biology of organic molecules, the physical chemistry of life, and artificial and model life, where we do not have enough internal

breadth. Over the five years of this proposal we would train 100 students, and make significant strides to develop a broad astrobiology program at the UA and to provide well-trained scientists for astrobiology endeavors at other institutions.

As noted above, the Astrobiology Roadmap and the COEL report have suggested that the Astrobiology Institute should be more concerned with the astronomical environment that shapes planetary systems. We believe that this is indeed essential to astrobiology. In the present proposal, we draw heavily upon our current strengths in astronomical research programs that relate directly (often unknowingly) to astrobiology, and we propose to broaden the scope of these to include many other astrobiology-oriented activities in the College of Science at the University. Further, we expect this program to encourage dedication of new faculty positions to areas where we have major gaps. This is consistent with the UA goals to place increased emphasis on development in life sciences.

I.6 Access to Telescope Facilities

The problem of incorporating more astronomy into the astrobiology activity has received much attention. It might naively be assumed that the need for astrobiology is widely accepted among astronomers, and all that is needed is to let astronomy into the astrobiology tent. Nothing could be further than the truth. It is clear that many in both astronomy and planetary sciences see broad based astrobiological studies as in competition with their more traditional work. The problem is greatest in the allocation of telescope time, which is essential to make progress on many of the Roadmap goals.

An example of this problem may be seen in the recent studies of earthshine to discover the nature of Earth's visible spectrum and help plan for Terrestrial Planet Finder like studies. There have been three requests to NASA facilities to study earthshine, two to HST and one to IRTF. All three proposals were rejected by telescope time allocation committees. In the same era, there were three requests for observing time at ground telescopes outside NASA control, by members of the groups that control those facilities, Steward Observatory and Apache Point Observatory. Those three proposals were accepted. The first study (Woolf et al 2001) showed that in predicting the spectrum of Earthshine we had failed to predict both the Rayleigh scattering of the atmosphere or the "red vegetation edge" due to reflection from land plants but not aqueous photosynthetic organisms. Turner (2003) showed that the identification of the red edge was correct by showing the difference between observing when the illuminated earth was substantially vegetated and when it was desert. Finally, Turnbull *et al.* (in preparation) show that the Rayleigh scattering study is likely affected by cloud cover, and gave a measured strength of the 0.94 micron water band, the strongest band in the region of the spectrum available to CCD detectors.

The above example is a demonstration that the astronomical facilities that will be made available to this work both at Steward Observatory and NOAO are urgently needed. The Laplace Center will provide the appropriate vehicle for this to occur.

I.7 Impact on NASA Missions

The COEL Committee also noted a need for greater astrobiology input to the planning of space missions. Thus:

" An important operational goal of astrobiology is to inform NASA missions with respect to the techniques and targets for the search for life elsewhere, and the search for clues to the steps leading to the origin of life on Earth"

The UA group has already made significant contributions to astrobiologically relevant space missions. For example, the initial suggestion for detection of terrestrial planets in the infrared, and the use of ozone as a biomarker was made by Angel, Cheng and Woolf (1986); the work was funded by a NASA grant for studies of advanced optics in space. The development of the concept for a Terrestrial Planet Finder interferometer was supported as part of the Ex-NPS study. The development of a concept for a Life Finder device was developed with funds from the NASA Institute for Advanced concepts. The first earthshine studies (see above) were made using funds from JPLs industrial study of different possible TPF missions. The one consistent theme through all of these is that the science part has been tacked on to what were supposedly engineering studies, rather than being supported in their own right. Direct support for the science must be provided if the science is to flourish. This is why linking our work to the Astrobiology Institute is necessary. It will be even more important in the future as, for example, detailed planning of the TPF program will require major input from astronomical studies of the nature of exo-planetary systems. The Laplace Center can bring greater coherence to development of concepts for both astrobiology-related space sciences, which has been supported largely in an incoherent fashion. And the Tucson group can continue to make substantial contributions to this aspect of the NAI program.

I.8 The Proposed Research Program

As noted above our program is strongly oriented to the NAI need for greater connection with astronomy and builds on our strength in that area. As background we note that when TPF was conceived almost a decade ago, it was assumed that essentially all planetary systems had architectures like the solar system. Now, 104 more planets and 12 multiple planet systems later (<http://www.exoplanets.org>), we find that our solar system is unlike the other systems, and plans based on the idea of the solar system as the "typical" planetary system are being questioned. This impacts directly on fundamental questions of Astrobiology such as "Does life exist elsewhere in the universe?" and "How does life begin and evolve?"

In its broadest sense, astrobiology is not just a question of how life arose in a known environment such as Earth's. The chemical, physical and astronomical environment of early Earth is not well known. The origin of life on Earth is deeply linked to the question, "How typical is the Solar System?" If we try to put the Solar System into the context of the current information, including the recently discovered exo-planetary systems, it is possible to arrive at two wildly different conclusions. One is that earth-like planets are very common, and could be found by observing the environments of stars no more than 10 light years away. The second is that earth-like planets are so rare that only one or two are likely to exist in our entire galaxy. Obviously there is a flaw in at least one of these analyses! The answer is crucial to planning missions such as TPF.

It is generally agreed that the planetary systems being found by radial velocity studies are dynamically saturated, with little or no possibility of harboring rocky planets. Dynamical stability studies show that the relatively large eccentricities of the Jovian planets of these systems make retention of terrestrial planets in habitable zones nearly impossible over long time scales.

The conclusion that Earth-like planets are nonetheless common considers the radial velocity systems to be anomalous due to selection and rests on the observational result that the key ingredients of Earth's biosphere, rock materials and water are common in the galaxy. Laplace had hypothesized in the late 18th century that the planets of our solar system had formed from a disk of gas and dust orbiting the young Sun. The great strides in infrared astronomy in the last three decades have confirmed the basic picture of Laplace's model. Dusty disks are common around young stars in formation. The interpretation here is that *all* such disks form planets. The statistical argument is then made that the radial velocity systems cannot represent more than 20-30% of all stars and that these are the ones that did not retain earth-like planets. All others did form and retain earth-like planets, and so we should find them around most stars, even those in the immediate neighborhood of the sun.

The contrary conclusion obtains if one assumes that the planetary systems that are being observed with the radial velocity method are representative of all the planetary systems that form. We then calculate the fraction of those systems that would be like the solar system. Outside the regime where tidal forces circularize orbits, known extra-solar planets range widely in eccentricity, with their eccentricities uniformly distributed between 0 and 1. The solar system is very different. The eccentricities of the 8 main planets, Mercury through Neptune are all less than 0.5, and average 0.06. The probability that these arise from a uniform distribution from 0 to 1 is 6.6×10^{-10} . Then, because only < 25-30% of stars have planetary systems, the probability of a solar type star having a Solar System like ours is 1.6×10^{-10} . Since there are only $\sim 10^{10}$ solar type stars in our galaxy, there will be at most one or two systems.

Clearly we urgently need to discover the frequency of earth-like planets, both for the scientific interest in the issue, but also to plan future space missions such as Terrestrial Planet Finder. Either earth-like planets are essential for its goals, or the goals must change to discover the character of planetary systems. The concept of the mission is currently focused on the spectral regions where terrestrial planets will appear best, and so is not optimized for finding cool giant planets. We hope for the Kepler mission to discover the frequency of earth-sized planets in earth-like thermal environments by searching for the planets occulting their star. But those results would come very late to totally change the concept for a TPF mission.

Even if earth-like planets are common, there is still remains a crucial question, whether earth sized, earth temperature objects can be expected to be just rock spheres, or whether they may be expected to have volatiles, and so be habitable. Recent dynamical models suggest that the acquisition of volatiles by earths may be controlled by the masses and orbits of giant planets in the planetary system (Chambers 2003). If so will there be totally different environments where life might develop? On the other hand, even if Earths are rare, life could be abundant. One possible place for life to develop would be on the satellites of giant planets inside a star's habitable zone. The problem then becomes one of detecting life, and the problem of observing

satellites of a warm Jovian planet orbiting a star. These are beyond the range of current planet finder concepts. Thus it is important to learn as much now as we possibly can about how planetary systems form and develop.

Our research plan thus has a substantial effort focused on determining the character of extra-solar planetary systems. If systems like the solar system are not uncommon, there will be an abrupt increase in the frequency of giant planets at distances 5-10 times greater than the distances where an earth would form. We would expect to see signs of this in both the formation and development of planetary systems.

There are three facets of this problem where it can be explored observationally. First we can try to find out in young planetary systems where the planets are forming. This requires both low and high-resolution spectrophotometry of pre-planetary circumstellar disks. Spatial variations in the density of matter would indicate the characteristics of forming planets. Second we can study “second generation dust” in mature planetary systems. This dust is a product of collisions amongst minor planets (asteroids and Kuiper belt objects) and caused by the gravitational perturbations of massive planets. The spectral distribution of radiation from such a dusty debris disk will tell its temperature, and so its spatial distribution in the planetary system. Giant planets will sweep out dust-free zones. Thus observations of dust will tell where giant planets are present. The third method is to search for the planets themselves. We have been developing techniques for looking at such planets from the ground using adaptive optics and the novel approach of nulling interferometry. Large telescopes with adaptive optics are essential for this work and provided under this proposal. The Large Binocular Telescope is an ideal instrument and should be available for research for the majority of the 5-year period of this research.

The above paragraphs hopefully provide a useful background to the need for astronomical observations in the pursuit of astrobiology. Our proposed research program follows the likely time sequence of planetary evolution beginning with the most diffuse state of pre-planetary material and concluding with studies of planets themselves. Here we provide a brief summary of each of our three modules; details are to be found in sections 1, 2 and 3 respectively.

1.8.1 Module 1

In the first module we plan studies of prospective pre-planetary material in dense interstellar clouds and in circumstellar envelopes and disks, Our focus is on the search for complex organic molecules both to understand their prevalence, their formation processes and their ultimate impact on the materials available after planet formation. One key program involves the search for the presence of ribose in space. Ribose is a relatively simple organic molecule essential to the formation of ATP (adenosine triphosphate); ATP is the molecule used universally for energy storage and transport in all known biological processes. It is also a key ingredient in the monophosphate molecules that link together to form RNA and DNA The question of biological significance is why ribose is favored over other sugars the formation of which are energetically favored at higher densities (thermodynamically). On the other hand ribose formation is favored in conditions of kinetic control (low densities). The possibility that original ribose was formed by gas reactions in space rather than by aqueous reactions may solve a chicken-and-egg issue in the formation of RNA and DNA. We see in this an exciting possibility that nature may have jump-started life thus in the cosmos. This work will involve extensive laboratory efforts and follow up

observational work using the facilities of the UA Radio Observatories. We also plan to carry out a program of theoretical studies, backed by observational follow up on the formation of organic molecules in dense cores of interstellar clouds and circumstellar (especially carbon star) envelopes and in the interior of protoplanetary disks. This module addresses *Astrobiology goal 3.1*, sources of organic molecules and catalysts.

1.8.2 Module 2

In the second module, we plan several astrophysical studies related to the search for habitable planetary systems. We will study circumstellar dust disks as indicators of the presence and characteristics of giant planets, of the populations of minor bodies, and of the asteroidal and cometary bombardment history of terrestrial planets. The latter processes are dependent on the masses and orbits of planets in the system, and are significant for their effects both on the transport of volatiles across the system, and on habitability and the development of life. This study will address *Astrobiology goal 1.2* [direct and indirect observations of extrasolar habitable planets], *goal 1.1* [how solid planets acquire liquid water and other volatiles], and *Astrobiology goal 4.3* [effects of extraterrestrial events upon the biosphere].

We will also study the time-variability of sunlike stars. The high sensitivity of the earth's climate to the solar radiation received, and where it is received is well known. Solar changes have demonstrated severe effects on Earth's climate in the past, e.g. the “little ice age” that accompanied the Maunder sunspot minimum. Here we will examine how the current variability of the sun is likely to change if it follows the historical pattern of otherwise similar stars. We wish to quantify this to consider the effect of solar variation in early epochs, such as those in which photosynthesis developed, and in future epochs, to understand the effects of variability superposed on the continual brightening of the Sun. This study will also address *Astrobiology goal 4.3* as above, as well as *goal 6* [to understand the principles which will shape the future of life both on Earth and beyond].

1.8.3 Module 3

This module consists of searching for and studying planets with a view to establishing criteria for habitability. While the number of known exo-planetary systems (determined from radial velocity measures) now exceeds 100, there has to date been no direct detection of the radiation from a single extra-solar planet. This is clearly a problem in technology development, and we have included such a component in our program. We believe our experience and our record of innovation will lead to success in this area, and allow us to start characterizing planetary systems. Using the large telescopes available to the Laplace Center, we plan to develop and implement techniques for direct detection and (crude) spectroscopic analysis of planets around nearby stars.

A second component of this module is to advance our understanding, through modeling of the atmospheres of giant planets. This work will be an essential tool in interpreting the data expected from both ground-based and space observations during the next decade.

Also in this module is a component directed towards the study of radiation from the earth by further observations of earthshine on the moon. We have two goals for this work. The first is to make observations of earthshine in the spectral region between 0.8 and 2.3 microns. This is the

remaining unexplored region of the whole earth spectrum. Just as we discovered unexpected results in the visible spectrum, we are hopeful here. There are open questions on how the red vegetation edge feature changes with wavelength, and possible rock identification features that may show when desert regions dominate the field of view. We will also investigate how the visible/UV part of the spectrum changes with time, and attempt to interpret the spectrum, so as to be prepared for a Planet Finder mission.

Module 3 contributes to *Astrobiology goals 1.1 and 1.2*.

I.9 Management Plan The goal of our management plan (see section 4) is to ensure proper coordination of the Astrobiology node while maximizing the opportunities for the individual investigators to develop their ideas. The key to success will be communications. With the proper level of information flow and communication, coordination of the diverse science and educational elements will be straightforward.

Overall responsibility for the program will be the responsibility of the PI and Laplace Center Director, Neville Woolf. He will be assisted by Program Manager Tom McMahan and by Research module leaders, Lucy Ziurys, Steve Strom and Roger Angel. Michael Meyer will coordinate the Winter Institute and Tim Slater will lead the education and public outreach components.

The team plans regular internal meetings to assess progress and to fine-tune the research effort. It also plans close coordination with the NAI and with other NAI nodes.

I.10 Education and Public Outreach

Our EPO proposal (section 6) describes how we plan to strengthen astrobiology as an academic discipline and to provide opportunities for students to develop their interests in the field despite the barriers often presented by existing departments. It also contains an educational and public outreach component (EPO).

We have described above our plans for the Laplace Center. This will be the focus of an Interdisciplinary Program (IDP) at the University of Arizona. It will be run by a Director (initially Woolf) and will provide coordination of the entire Astrobiology node in Tucson. Members of the IDP will be drawn mainly from the current departments of Astronomy, Chemistry (and Biochemistry) and Planetary Sciences and from NOAO; it will be open to faculty members from other departments. The UA has a successful record in multi-departmental, multi-college IDPs, including those in Applied Mathematics and in Neurosciences. IDP programs of study will be developed so that students can earn academic qualifications within the IDP including minors in any of the departmental specializations of vice-versa. The initial focus will be on departments within the College of Science and the Winter Institute.

The Laplace Center will also coordinate interchange of faculty with other members of the NAI to develop understanding of issues in all areas of the roadmap. Some of this interchange will focus on the Winter Institute, which has been described briefly above and will also be coordinated by the Laplace Center. Students will not only participate in formal class work and seminars on astrobiology, but will be actively involved in both the astronomical, instrumental and laboratory activities described in I.8.

On the education side we will ensure that astrobiology components are available in the UA General Education programs in Natural Sciences - that is science for non-specialists. Astrobiology is a good topic for capturing interest as a general science education topic for undergraduate students in non-science fields. Much of the student enrollment Natural Sciences is in the Astronomy and Planetary Sciences departments, which together provide instruction for over 1,500 students per semester. The Laplace Center will ensure that suitable astrobiology materials are available for these and similar courses in Geosciences, the Tree Ring Lab, Ecology and Evolutionary Biology.

In our EPO program, we have an integrated education and public outreach component. EPO Lead T.F. Slater's primary area of scholarship is the teaching and learning of astronomy and geosciences. He is a member of the College of Science high school science teacher preparation program, the director of the UA Science and Mathematics Education Center and an associate professor of astronomy at UA. His astronomy education research group focuses on identifying students' misconceptions in astronomy and designing effective instructional materials to improve student understanding, both in formal courses and for museums and informal science centers. This unique research group has earned national recognition in the area of astrobiology education by conducting seminal research that systematically studies student beliefs and reasoning difficulties regarding the search for life in the universe. This work serves as the foundation for a new laboratory activities manual for undergraduate astrobiology courses for non-science majors. Dr. Slater is also working with Discovery Park, a science education center located in Safford, Arizona at the foot of Mt. Graham. His goal is to use the center and the proximity of major astronomical facilities on Mt. Graham to extend the outreach program to parts of rural Arizona and to the San Carlos Indian reservation. The Laplace Center will provide material and support to these efforts.

In addition Dr. Don McCarthy has, for many years, run a very successful Astronomy Camp for high school and university students as well as for teachers using the astronomical facilities on Mt. Lemmon and incorporating components of geosciences and tree ring studies as well as astronomy. If selected, the Laplace Center will seek to expand this activity and to ensure that suitable materials on astrobiology are available for each of the above program elements.

1. Module 1: The Building Blocks of Life: Astrochemistry of Simple Sugars and Other Prebiotic Molecules

Team: L. Adamowicz, A. Apponi (Deputy), M. Brown, D. Halfen, E. Herbst, R. Polt, L.M. Ziurys (Lead).

1.1 Introduction

The key life processes of metabolism and reproduction have a related chemistry. The breakdown of intake proteins into amino acids is achieved by hydrolysis, and the reconstruction of desired proteins requires a condensation reaction in which energy is required to put more water into the aqueous solution. This energy comes from the conversion of ATP (adenosine triphosphate) into ADP (adenosine diphosphate). The reproductive helices of RNA and DNA are constructed from the monophosphates of adenosine (AMP), guanosine (GMP), etc. Common to both of these biological processes is Nature's exclusive use of pentose sugars, namely ribose and deoxyribose, in the structures of all nucleotides. The origin of ATP, ADP and AMP from prebiotic material is obscure since reproduction of them requires both helix formation and condensation reactions. In space, the presence of simple sugars and important organic molecules is made possible because ion-molecule and other low-barrier reactions are achieved in a space medium. In this module we explore the possibility that ribose forms in space, is collected into comets and primitive meteorites and falls to earth, into an appropriate version of Darwin's warm pond, acting to jump-start life processes. Theoretical modeling of pathways leading to interstellar ribose is also discussed, as well as calculations of abundances of complex molecules both in molecular clouds and protostellar disks. In addition, we express the possibility of formation of organized nanostructures, which may function as prebiotic membrane systems. This study therefore belongs to objective 3.1 of the astrobiology roadmap.

1.2 The Investigation of Interstellar Molecules: Beginnings of Astrochemistry

The field of astrochemistry really began in 1963 when the lambda-doubling transitions of the OH radical were detected at 18 cm towards dense gas in Casseopia A, a supernova remnant (Weinreb et al 1963). This species was the first interstellar molecule observed at radio wavelengths. Up to that time, it was generally thought in astronomy circles that the gas between the stars, the so-called "interstellar medium," was, at its densest, only 10-15 particles per cm³. Given this low

Table 1.1. Known Interstellar Molecules

2	3	4	5	6	7	8	9	10		
H ₂	CH ⁺	H ₂ O	C ₃	NH ₃	SiH ₄	CH ₃ OH	CH ₃ CHO	CH ₃ CO ₂ H	CH ₃ CH ₂ OH	CH ₃ COCH ₃
OH	CN	H ₂ S	MgNC	H ₃ O ⁺	CH ₄	NH ₂ CHO	CH ₃ NH ₂	HCO ₂ CH ₃	(CH ₃) ₂ O	CH ₃ (C≡C) ₂ CN
SO	CO	SO ₂	NaCN	H ₂ CO	CHOOH	CH ₃ CN	CH ₃ CCH	CH ₃ C ₂ CN	CH ₃ CH ₂ CN	(CH ₂ OH) ₂
SO ⁺	CS	NNH ⁺	CH ₂	H ₂ CS	HC≡CCN	CH ₃ NC	CH ₂ CHCN	C ₇ H	H(C≡C) ₃ CN	
SiO	C ₂	HNO	MgCN	HNCO	CH ₂ NH	CH ₃ SH	H(C≡C) ₂ CN	H ₂ C ₆	H(C≡C) ₂ CH ₃	
SiS	SiC	SiH ₂	HOC ⁺	HNCS	NH ₂ CN	C ₅ H	C ₆ H	CH ₂ OHCHO	C ₈ H	11
NO	CP	NH ₂	HCN	CCCN	H ₂ CCO	HC ₂ CHO	c-CH ₂ OCH ₂	HC ₆ H		H(C≡C) ₄ CN
NS	CO ⁺	H ₃ ⁺	HNC	HCO ₂ ⁺	C ₄ H	CH ₂ =CH ₂	H ₂ CC(OH)H			
HCl	HF	NNO	AiNC	CCCH	c-C ₃ H ₂	H ₂ C ₄				12
NaCl	SH	HCO	SiCN	c-C ₃ H	CH ₂ CN	HC ₃ NH ⁺				C ₆ H ₆
KCl	HD	HCO ⁺	SiNC	CCCO	C ₅	C ₅ N				
AlCl	FeO ⁺	OCS	H ₂ D ⁺	C ₃ S	SiC ₄	C ₅ S?				13
AIF		CCH	NH ₂	HCCH	H ₂ C ₃					H(C≡C) ₅ CN
PN		HCS ⁺	KCN?	HCNH ⁺	HCCNC					
SiN		c-SiCC	SiH ₂ ?	HCCN	HNCCC					
NH		CCO		H ₂ CN	H ₂ COH ⁺					
CH		CCS		c-SiC ₃						
				CH ₂ D ⁺ ?						

15 ions
6 rings
~100 Carbon Molecules
19 Refractories

Total = 134

density, and the presence of a strong ultraviolet radiation field from background stars, it seemed unlikely that anything more than a few diatomic molecules could exist in interstellar gas. This assumption was supported by observations at the time, primarily 21 cm and continuum radio astronomy, which showed that large amounts of hydrogen atoms (“HI”, in astronomy terms), and ionized hydrogen (H^+ or HII) existed throughout the galaxy. Observations at optical wavelengths did result in the detection of a few diatomic species, such as CH^+ , CN, and CH (e.g. Adams 1948), which were observed in diffuse gas in absorption against background stars. The dusty regions of “dark clouds” that often obscured measurements of optical astronomers were usually ignored, that is, until the discovery of OH. Several years later, NH_3 , H_2O , and H_2CO were also detected at radio wavelengths (1.2 cm and 6 cm) by Cheung *et al.* (1968) and Snyder *et al.* (1969), added to the inventory of interstellar compounds. The largest breakthrough in astrochemistry occurred in 1970, when Wilson *et al.* (1970) observed emission from carbon monoxide from the Orion Nebula at 3 mm, using the NRAO 36 ft. radio telescope (now the 12 m). This unique discovery and years of subsequent observations have shown that the CO molecule is abundant and ubiquitous throughout the Milky Way Galaxy. Moreover, emission from this species is very intense and readily detected. In addition, these measurements showed that molecular emission was easily observed at short radio (i.e. millimeter) wavelengths. In fact, following 1970, there was very rapid progress in the identification of new interstellar compounds, primarily at millimeter wavelengths. The list continues to grow. Currently, there are over 120 securely identified unique interstellar molecules as shown in Table 1.1.

Contrary to earlier notions, the interstellar medium is sufficiently dense to support a complex chemistry. This chemistry occurs throughout the Galaxy, and even in external galaxies. This fact is illustrated by recent “all-sky” surveys of certain species such as carbon monoxide, as shown in Figure 1.1. This figure shows a plot of CO, $J = 1 \rightarrow 0$ spectral line emission (peak intensity) versus position across the galaxy, overlaid across the optical picture of the Milky Way.

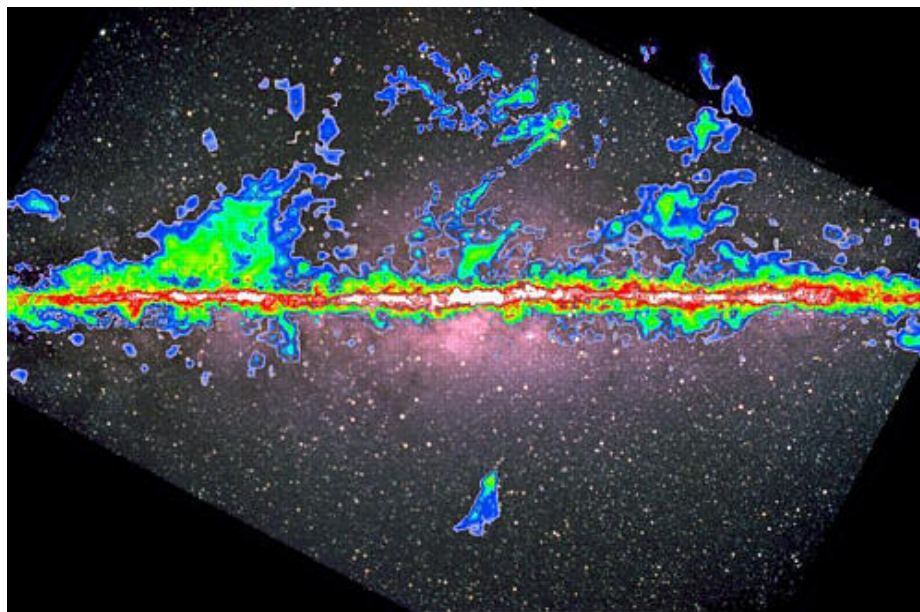


Figure 1.1. The “Molecular Milky Way:” a plot of CO, $J = 1 \rightarrow 0$ spectral line emission at 115 GHz (3 mm) as a function of position, illustrating the predominance of molecular gas. In the background is the optical picture of the Galaxy.

Relative intensity is shown as a color scale, white indicating the strongest emission. The figure illustrates the molecular gas is present in most regions where stars exist, but also in areas far from the galactic plane.

Astronomy conducted at millimeter (0.3-3 mm) wavelengths has therefore been a primary tool of interstellar chemistry, not only for the discovery of new molecular species, but also in examining their abundances and distributions in the Galaxy. Millimeter astronomy has distinct advantages for studying such molecules because the spatial resolution at these wavelengths matches the sizes of molecular emission on the sky. Also, quantum mechanics favors millimeter wavelengths. Because most dense gas in the interstellar medium is cold, with temperatures $T_k \sim 10 - 100$ K, in general only the rotational energy levels of a molecule are populated, as opposed to vibrational and electronic. Hence, interstellar species are identified on the basis of their “pure rotational spectrum,” which occur primarily at millimeter wavelengths.

Emission lines are produced by collisions, primarily with H_2 , which excite higher rotational levels, followed by spontaneous decay. Collisional excitation in colder gas therefore means that linewidths of interstellar emission features are very narrow, typically 1 part in 10^6 . Hence, the spectra obtained from interstellar gas are “high resolution,” such that not only are individual rotational transitions well defined, but fine and hyperfine structure as well. Hence, interstellar molecules can be securely identified on the basis of their “fingerprint” patterns. Illustrations of such patterns are shown in Figures 1.2. Given sufficient measurements, followed by a knowledgeable spectral analysis, a given chemical compound can be identified in interstellar gas beyond any doubt.

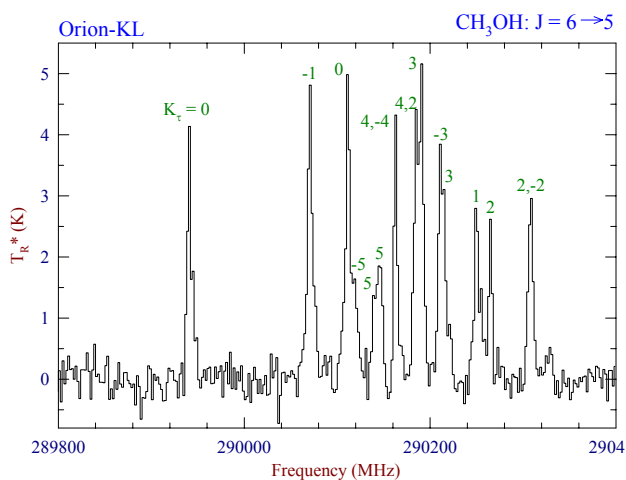


Figure 1.2a. Spectra of the $J = 6 \rightarrow 5$ transition of methanol (CH_3OH) observed toward the Orion molecular cloud near 290 GHz (1 mm). Individual features arise from “K- structure,” the pattern, which is unique to methanol, is based on its molecular weight and geometry.

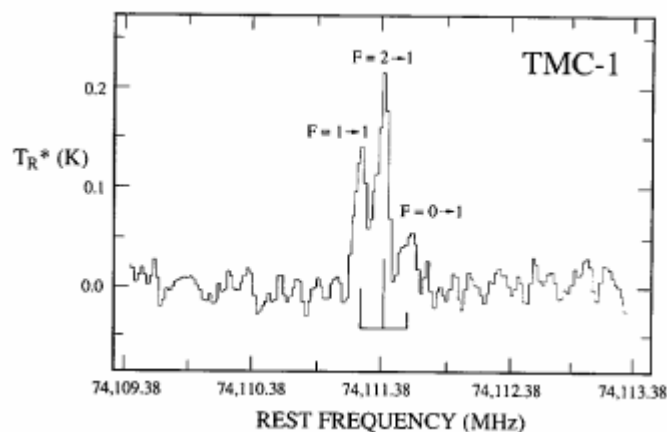


Figure 1.2b. Spectrum of the $J = 1 \rightarrow 0$ rotational transition of $HCNH^+$, observed at 74 GHz towards the Taurus molecular cloud. The three separate features arise from nuclear quadrupole splittings due to the nitrogen (^{14}N) nuclear spin. This unique “hyperfine” structure serves as a fingerprint for $HCNH^+$.

A key ingredient to the study of interstellar molecules has been laboratory spectroscopy. The spectral signature of a new species must be known before it can be identified in interstellar gas.

This fact has become particularly clear as millimeter astronomy achieved higher sensitivities through advanced detector development. It is very common that, in addition to known spectral features, any sensitive observation at millimeter or sub-millimeter wavelengths will contain so called “U-lines,” i.e., unidentified lines. These are emission features arising from yet to be discovered interstellar compounds. Currently, hundreds of U-lines are known to arise from the Orion molecular cloud alone; a small subset is shown in Figure 1.3. Amazingly, not one of these spectral lines can be securely identified, although one may arise from ethanol and two others from methyl formate. The common appearance of U-lines in interstellar spectra means that chance coincidences are not unusual. Consequently, the pure rotational spectrum of any proposed new molecule must be very accurately measured in the laboratory (1 part in 10^7 - 10^8) over a large wavelength region. Direct measurements in the lab are preferable, but extrapolated predictions, in particular to higher frequencies (i.e. higher rotational levels) can be reliable as well, provided sufficient lower frequency measurements are made such that all the necessary spectroscopic constants are well characterized. Current laboratory techniques in the rotational regime, such as direct millimeter-wave absorption spectroscopy (e.g. Hirota 1985, Ziurys *et al.* 1994) and Fourier transform microwave methods (Balle & Flygare 1981) are extremely powerful and have both the sensitivity and resolution to tackle most astrophysical problems.

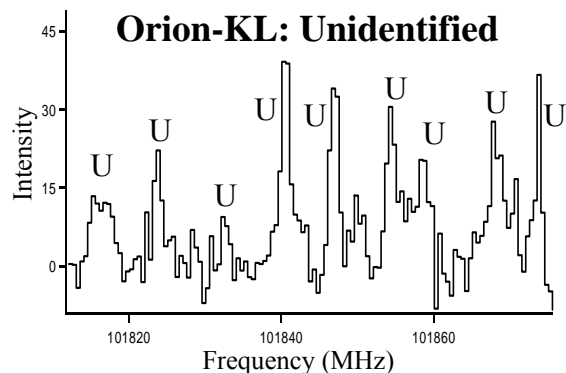
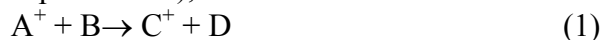


Figure 1.3. Unidentified emission lines observed towards the Orion molecular cloud near 101 GHz. Such features remain a puzzle for astronomer and spectroscopist alike.

1.3 Organic Chemistry in the Gas-Phase: Towards Greater Chemical Complexity

The current compendium of interstellar compounds clearly demonstrates that the chemistry in space is primarily organic. Not only do 75% of the known species contain carbon, but also all the basic organic functional groups are present. For example, the carbonyl group is represented by common species like formaldehyde ($\text{H}_2\text{C}=\text{O}$) and acetone ($\text{CH}_3)_2\text{C}=\text{O}$). There are various amides (NH_2CH_3 , NH_2CN), acids (HCOOH , CH_3COOH), and many compounds with the CN moiety (HCN , HC_3N , HC_5N , CH_3CN , EtCN , etc.) Basic aldehydes, ketones, esters, and ethers are additionally present. Some representative organic compounds are shown in Table 1.2.

The basic mechanisms thought to form organic interstellar molecules are two-body ion-molecule reactions (e.g. Herbst and Klemperer 1976), of the basic form:



These processes were initially postulated because they usually have no activation barriers and proceed at the collisional (or Langevin) rate ($k \sim 10^{-9} \text{ cm}^3 \text{ s}^{-1}$). Hence, they can readily proceed at the low temperature ($T_K \sim 10$ -100 K), low density ($n \sim 10^3$ - 10^6 particles/ cm^3) environment of interstellar clouds, where 3-body collisions do not occur and reactions with normal neutral-neutral type barriers would never occur. Chemical modeling has shown (Lee, Bettens & Herbst 1996) that ion-molecule reactions can produce the more complex species within the postulated lifetime of a molecular cloud ($10^6 - 10^7$ years), including dimethyl ether, methyl formate and

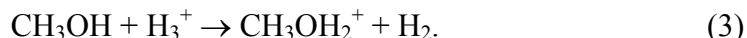
ethanol. For example, methyl formate can be created via the reaction (Millar, Herbst and Charnley 1991):



Neutral methyl formate is then produced by:



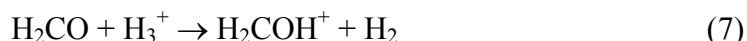
This process is quite viable because both H_2CO and CH_3OH have large interstellar abundances (e.g. Minier & Booth 2002). The ion CH_3OH_2^+ could be created by the process:



H_3^+ is the dominant ion in an astrophysical plasma, and it is readily created from H_2 and cosmic rays from the sequence:

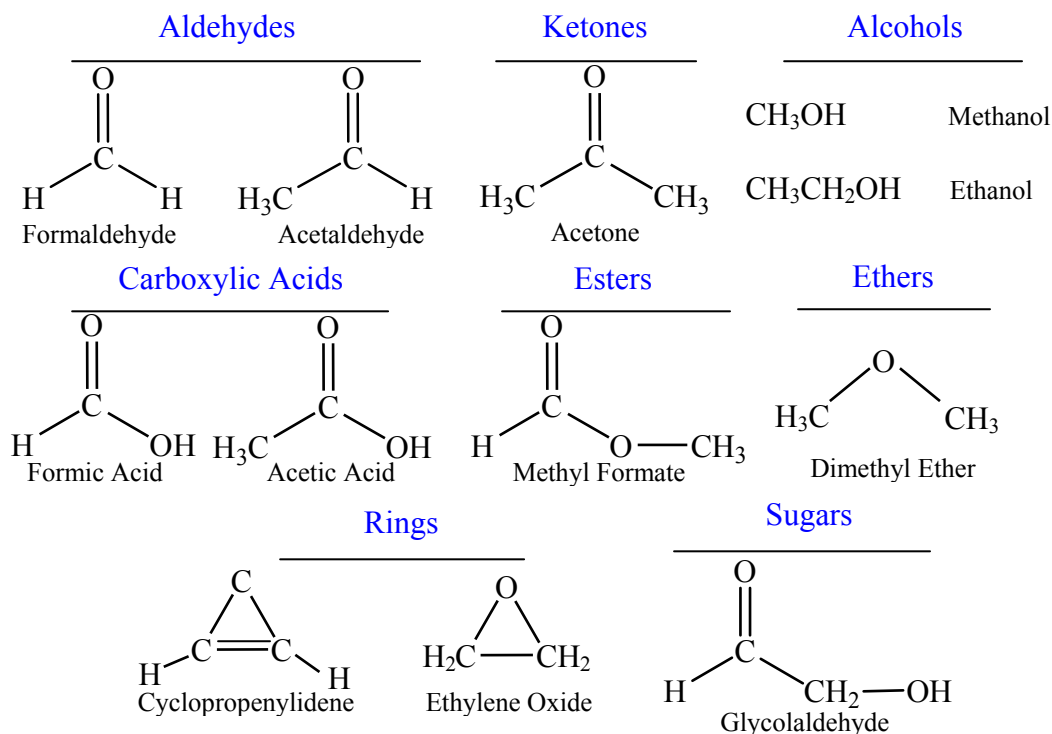


Because H_2 is the most abundant interstellar molecule and cosmic rays are common, large amounts of H_3^+ must exist in dense gas. There is sufficient H_3^+ for many types of proton transfer processes. Some common reactions are:



Given the relatively large abundances of HCO^+ and H_2COH^+ in interstellar clouds (e.g. Ohishi *et al.* 1996), these reactions must occur.

Table 1.2: Interstellar Organic Molecules



It is clear that as millimeter-wave telescope systems become more sensitive, more complex organic species are being found in the gas phase in interstellar space. Acetone and acetic acid, the next step in complexity from formaldehyde and formic acid, for example, have just recently been identified (Ramijan *et al.* 2002; Snyder *et al.* 2002). Such compounds, of course, are very simple in comparison to proteins or even sugars. However, given the observation of large numbers of unidentified features in interstellar spectra, and the fact that millimeter telescopes can do ever increasingly sensitive measurements, it would seem to be self-evident that the complexity of detected interstellar compounds will increase. The fundamental question is, what are the limits for gas-phase interstellar chemistry? Can it produce molecules of sufficient complexity to be of biological significance? In other words, are the building blocks of life present already in interstellar gas clouds?

1.4 Interstellar Ribose: A Likely New Species?

Although there are many biologically important molecules, perhaps one of the most fundamental is DNA and its single-strand counterpart, RNA. Together, DNA and RNA are responsible for storage, transport, and expression of genetic information. DNA, or deoxyribonucleic acid, is a double-stranded polymer consisting of repeating nucleotide units. Each nucleotide contains a phosphoric acid group, the pentose β -D-2-deoxyribose, and a purine or pyrimidine base. An example of such a nucleotide is shown in Figure 1.4.

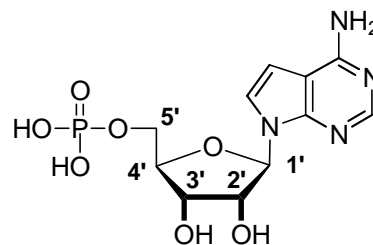


Figure 1.4: Adenosine 5-monophosphate, otherwise known as AMP, one of the nucleotides that forms RNA.

The two strands that form DNA, the so-called “double helix,” attach to each other via hydrogen bonds between the nucleotide bases. Such bonds are possible only between certain base pairs, such as cytosine and guanine, or adenine and thymine. RNA, or ribonucleic acid, is often single stranded, with the pentose in this case being β -D-ribose, with the base uracil replacing thymine. The individual nucleotides bond together via the pentose in both RNA and DNA; the linkages are made between the 3' and 5' carbons of the pentose using a phosphate (P-O-C) bond.

Ribose and deoxyribose are thus critical to the structures of RNA and DNA. They are both 5-membered rings consisting of four carbons and one oxygen atom. The fifth carbon is attached to

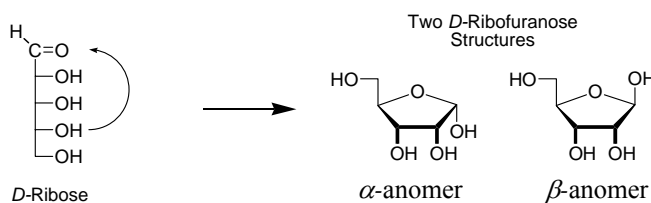


Figure 1.5: Cyclization of *D*-ribose leads to the two anomeric ribofuranosides, thus preventing further chain extension *via* the formose reaction.

the ring at the 4' carbon. Structures for these compounds are given in Figure 1.5.

To appreciate the structures of these pentoses, it is useful to consider that of monosaccharides in general. The simplest monosaccharides are trioses, which contain three carbon atoms. Examples of trioses are L- and D- glyceraldehyde. These species are chains as opposed to rings, and they have one chiral center and hence, two enantiomers, D and L, which are mirror images of each other.

Four carbon sugars (tetroses) also have chain geometries with two chiral centers and four stereoisomers. By the time pentoses form, i.e. five carbon sugars, the structures are large enough such that the most stable geometry is cyclic, generating four chiral centers and 16 stereoisomers. Cyclization of these compounds prevents further chain extension. The α - and β - designations refer to the orientation of the C-1 OH group relative to the other functional groups on the ring. All naturally occurring sugars on Earth are D-sugars; similarly all protogenic amino acids exist as a single antipode (L-isomers, e.g. Engel & Macko 1997).

Ribose and deoxyribose are certainly not large biological molecules, indicative of life. On the other hand, they are essential for life as we know it. Detection of these molecules in the interstellar gas would certainly revolutionize our thinking about where and how life began. Ribose could in fact be synthesized in space from ion-molecule reactions, as is postulated for other smaller organic compounds. Sugars in the terrestrial laboratory are readily synthesized via the formose reaction, which is the successive base-catalyzed addition of formaldehyde, H_2CO , (Butlerow 1861). By analogy, sugars could be formed in interstellar space via successive additions of protonated formaldehyde, H_3CO^+ , a common interstellar molecule. Because of the high vacuum conditions, an acid-catalyzed process is feasible in space. The starting materials could be glycolaldehyde ($\text{CHO}-\text{CH}_2\text{OH}$), or *cis*-1,2-dihydroxyethylene ($(\text{HO})\text{HC}=\text{CH}(\text{OH})$), which are enol-keto tautomers with the keto form more stable by $15.4 \text{ kcal mol}^{-1}$ (Su *et al.* 1999). There is some evidence that glycolaldehyde may be present in interstellar gas from the work of Hollis, Lovas and Jewell (2000). (The laboratory spectrum of this species is known, unlike the latter molecule.) Either species could react with H_3CO^+ via a radiative association ion-molecule process, which should occur relatively rapidly in the interstellar environment, resulting in the protonated form of the desired sugar:



This reaction can occur quickly because the large protonated complex can be stabilized through vibrational channels (Petrie 1996). The neutral molecule can be formed in a number of ways; for example, by recombination with an electron, proton transfer with H_2 or CO , etc.



The sugar glyceraldehydes can thus be synthesized, either the D or L forms. The addition of H_3CO^+ to glycolaldehyde could also result in other products, such as dihydroxyacetone and several keto-sugars. Glyceraldehyde is a triose; formation of tetrose sugars would occur by the addition of H_3CO^+ to the trioses. Addition to D-glyceraldehyde would create D-erythrose and D-threose. From D-erythrose, the next addition would result in D-ribose and D-arabinose. This

synthetic scheme is presented in Figure 1.6. Deoxyribose could be produced from D-erythrose, as well in a fashion analogous to that depicted in reactions (8) and (9).

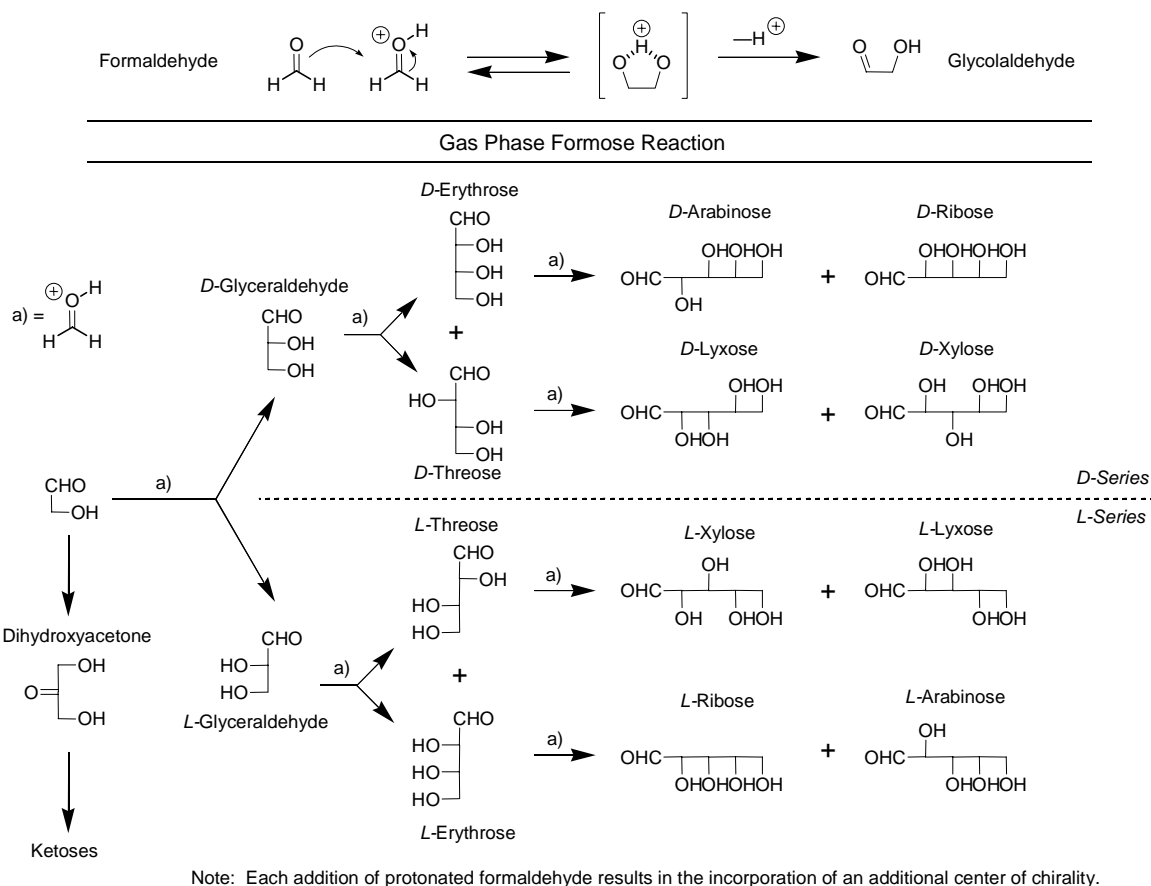


Figure 1. 6. Production of D-ribose from glycolaldehyde via ion-molecule addition of H_3CO^+

There are other possible schemes leading to the creation of sugars besides the one proposed here. For example, certain neutral-neutral reactions might be involved in the scheme, or other ion-molecule reactions. The point of this exercise is to show that ion-molecule chemistry in principle could produce sugars as large as ribose. Several organic ring species are already known to exist in interstellar gas (C_3H_2 , $\text{C}_2\text{H}_4\text{O}$). These are three-membered rings, and therefore, should suffer more strain than larger structures. It is suggested that the process could be inhibited at the 5-carbon (ribose) stage because cyclization would remove the aldehyde functionality necessary for the formose reaction to proceed to a 6-carbon sugar.

If ion-molecule type reactions produced ribose and deoxyribose, this formation process would be kinetically rather than thermodynamically controlled. Studies by Eschenmöser and collaborators (e.g. Wilds *et al.* 2002) suggest that sugars other than ribose are just as likely to form RNA-like structures. In fact, the capability of Watson-Crick base-pairing is widespread among potentially natural nucleic acid alternatives that are close in structure to RNA (Eschenmöser 1999). Why then D-ribose, and not another isomeric pentose? This remains an open question. It could well be that the structure of RNA resulted from synthetic contingency, not from combinatorial generation and functional bias. Ion-molecule chemistry might selectively generate ribose as the primary pentose, providing exactly this contingency. Experiments have indeed shown that ribose is preferentially formed in kinetically controlled aldolization reactions (Müller *et al.* 1990).

Kinetically controlled interstellar chemistry could be guided by the same molecular forces, i.e. dipole-dipole interactions and hydrogen bonding).

If reaction rates were known for the ion-molecule processes leading to ribose, then this problem could be readily attacked. However, these rates are not known, and it would take a long-term experimental endeavor to actually measure them at interstellar temperatures. On the other hand, identifying ribose and its simpler sugar precursors in interstellar gas would be highly suggestive that gas-phase chemistry preferentially provided the starting materials for RNA, especially if other pentose alternatives were not found, or found in lesser abundance.

The purpose of this section of the proposal is to carry out systematic searches for ribose and its sugar precursors in interstellar gas using the highly selective techniques of high-resolution spectroscopy and radio/mm astronomy. These combined methods are so exact that with careful, thorough studies, the existence of these compounds in interstellar space can be established beyond any shadow of a doubt, as in the case of other interstellar molecules. To carry out this program, however, extensive laboratory spectroscopy must be completed first. Of the precursors proposed for ribose in Figure 1.6, only the pure rotational spectrum of glycolaldehyde has been measured with sufficient accuracy with a large enough data set for meaningful interstellar measurements. Some of the species of interest include hydroxyacetone, dihydroxyacetone, D-glyceraldehyde, D-erythrose, D-threose, D-xylose, D-ribose, and D-lyxose. A new absorption spectrometer will be built to study these molecules in a wavelength range comparable with their most intense rotational transitions (~10-100 GHz). Once the necessary laboratory studies have been completed, a search for each molecule will be conducted in interstellar gas using the University of Arizona's two radio telescopes, the Kitt Peak 12 m, and the Sub-mm telescope (SMT). These facilities are operated by the Arizona Radio Observatory (ARO); the director is a co-PI on this proposal. Large amounts of telescope time will have to be devoted to searching for such molecules. The ARO is committed to providing this time, if this proposal is funded. Because the proposed molecules are large species, by interstellar standards, they will have hundreds of favorable rotational transitions across the millimeter spectrum. This plethora of lines will be measured and analyzed as a complete data set to avoid fortuitous coincidences with other species, and to secure an accurate identification. Our computational group will carry out theoretical investigations in parallel to establish which interstellar processes could actually lead to sugars and other complex species.

1.5 The Astrochemistry Team

The astrochemistry team consists of three expert high resolution molecular spectroscopists (Ziurys, Apponi & Herbst, who is very experienced in the analysis of organic molecules with complicated spectra), two theorists (Adamowicz & Herbst), who will explore the interstellar pathways for formation of the sugars and examine abundances of large organic molecules in dense clouds and protostellar disks, one synthetic organic chemist (Polt), who will provide the necessary precursors for the lab work and bioorganic interpretations of interstellar mechanisms, and one biochemist (Brown), who will interpret the implications of these results for RNA and DNA structure. In addition, three members of the team are highly experienced radio observers who have discovered numerous other interstellar molecules (Ziurys, Apponi & Halfen).

In the next sections, the laboratory spectroscopy, radioastronomical observations, theoretical calculations, and work with condensed membrane systems will be discussed in more detail.

1.6 Laboratory Spectroscopy of Proposed Interstellar Sugars

1.6.1 Experimental Apparatus

The spectrometer to be designed is a classic absorption experiment consisting of a radiation source, an absorption cell with a supersonic jet nozzle for molecular cooling, and a sensitive microwave detection system. This instrument will be designed to operate over a frequency range of 10 – 110 GHz where the signals from the species of interest are expected to be the strongest. For example, at an operating temperature of 50 K (a result of jet cooling), the spectrum of glyceraldehyde exhibits its peak intensity near 89 GHz (see Figure 1.8). Although the spectrometer as a whole is not commercially available, most of the individual parts can be purchased from commercial vendors, and these parts will be discussed in the following four sections.

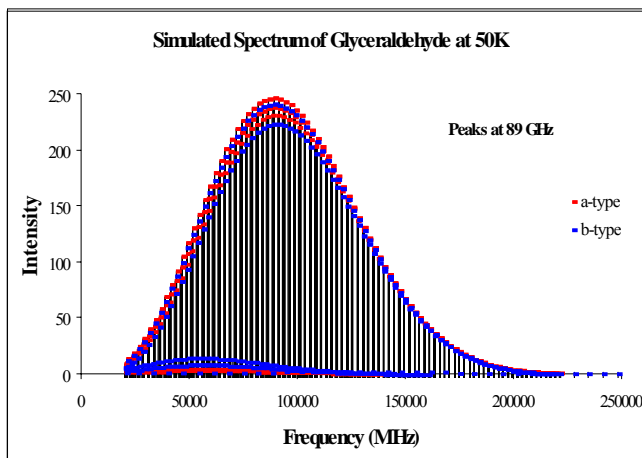


Figure 1.7. Calculated intensities for the individual rotational transitions of glyceraldehydes at 50 K.

Radiation Source:

The radiation source for this experiment will be a low phase noise, high power Agilent E8247C series signal generator operating in the frequency range of 250 kHz – 40 GHz. Phase-locked Gunn oscillators will be used to generate frequencies higher than 75 GHz, which we already have in our laboratory.

Absorption Cell and Optical Components:

A diagram of the gas cell is shown in Figure 1.9. The cell will be approximately 0.30 m × 0.60 m, and will be evacuated by a Varian VHS-10 (5300 liter/s) oil diffusion pump equipped with a Leybold D65B (53 cfm) roughing pump, creating a vacuum of better than 10^{-7} torr. The supersonic beam expands perpendicular to the radiation, and the molecules are terminated on a liquid nitrogen cooled Chevron baffle to help reduce contamination in the pump oil. The radiation will be launched from tapered feedhorns and focused to a waist of about 2 cm at the center of the cell where absorption by the molecules will occur. The radiation is then allowed to pass out of the cell and is refocused onto the detector (see Figure 1.9).

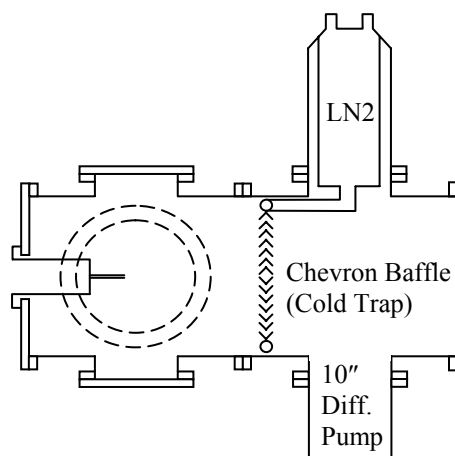


Figure 1.8. Elevation sectional view of vacuum chamber used for free-jet microwave spectroscopy

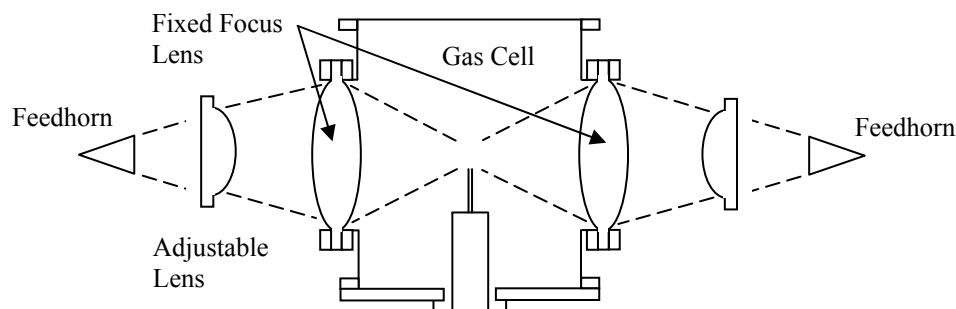


Figure 1.9. Top sectional view of gas cell. Dashed lines show the propagation of the microwave radiation.

Molecular Beam Apparatus:

The supersonic jet will be produced from a continuous flow or pulsed nozzle as shown in Figure 1.10.

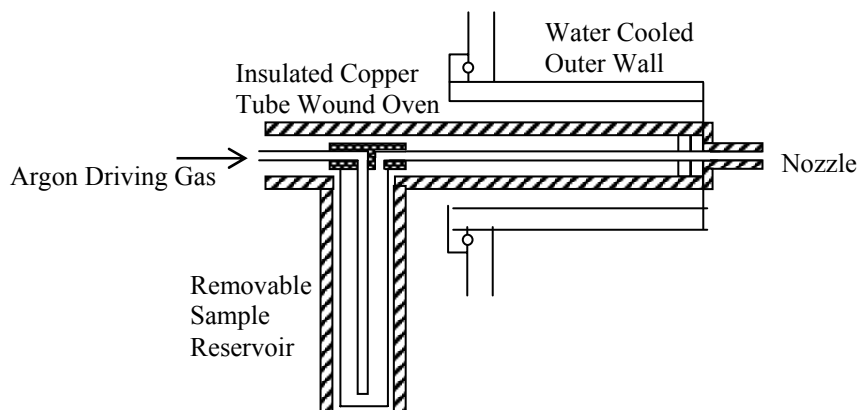


Figure 1.10. Water cooled insert to main chamber showing sample inlet and nozzle layout.

Detection System:

A standard phase sensitive detection scheme will be employed for this experiment incorporating a liquid He cooled (4.2K) InSb hot-electron bolometer (Cochise Instruments). The radiation source will be frequency modulated at a 20 – 50 kHz rate and demodulated by a lock-in amplifier. Data acquisition will be under computer control via GPIB interface.

1.6.2 Proposed Molecules

High-resolution spectra will be obtained from this system on the large molecules proposed (see Table 1.3). Sensitive searches over large frequency ranges are necessary to positively identify these species. The advantage of this system over many other microwave and millimeter wave systems is that automated data taking is possible without user intervention. Samples in the oven are expected to last for many hours, possibly overnight, without being exhausted. High-resolution spectra will be recorded using this technique with linewidths <100 kilohertz, and measured frequencies will be accurate to a few kilohertz—necessary for assignment of the interstellar spectrum. Unlike vibrational or electronic spectroscopy, rotational spectroscopy offers an unambiguous assignment of the molecular species where each measured line is unique to a given species. Each line measured, however, is like a piece in a puzzle that the spectroscopist must first assemble in the laboratory with limited contamination before attempting to assign the complicated interstellar spectrum.

Initial work will be done on the smaller molecules, 1,2-dihydroxyethylene, and hydroxyacetone; then the spectra of the larger sugars, dihydroxyacetone, D-glyceraldehyde, D-erythrose, and D-ribose, will be measured. Analysis of these data for the sugar molecules proposed will yield

Table 1.3: Proposed Laboratory Species

Molecule	Ground State	Estimated Constants (GHz)			Dipole Moment	Commercially Available Form
		A	B	C		
1,2-Dihydroxyethylene	1A	26.56	2.16	1.99	a, b-types	Must Synthesize
Hydroxyacetone	1A	10.34 ^a	3.82 ^a	2.86 ^a	a, b-types	Solid Dimer
Dihydroxyacetone	1A_1	4.73	1.86	1.33	b-type	Solid Dimer
D-Glyceraldehyde	1A	~3.0	~1.8	~1.2	a, b, c-types	80% in Solution
D-Erythrose	1A	~2.0	~1.2	~0.8	a, b, c-types	Pure Syrup
D-Threose	1A	~1.8	~1.4	~0.8	a, b, c-types	60% Syrup
D-Xylose	1A	~1.0	~0.8	~0.4	a, b, c-types	Pure Solid
D-Arabinose	1A	~1.0	~0.8	~0.4	a, b, c-types	Pure Solid
D-Lyxose	1A	~0.9	~0.9	~0.4	a, b, c-types	Pure Solid
D-Ribose	1A	~1.1	~0.7	~0.4	a, b, c-types	Pure Solid

^a Experimentally determined by Kattija-Ari, & Harmony (1980)

spectroscopic constants for these species. The rotational constants, A, B, and C, as well as centrifugal distortion constants will be determined from their spectra. Significant K-ladder structure will be observed, which will establish the spectroscopic constants to high accuracy, which is necessary for subsequent astronomical searches.

1.7 Astronomical Observations:

To detect the proposed compounds in space, high sensitivity searches will be conducted; primarily at the Kitt Peak 12m telescope. This instrument is, in fact, currently being used to confirm the presence of glycolaldehyde in interstellar gas in the Galactic center in a source called “Sgr B2(N).” Some confirming spectral lines are shown in Figure 1.12. The measurements will be primarily conducted in the 3 mm and 2 mm bands (65-180 GHz). The objects to be studied include a variety of Galactic dense molecular clouds, such as Sgr B2 (Galactic center), the Orion molecular cloud, W51, W49, NGC7538, DR21(OH) and G34.3. These sources are known to contain star forming regions and hence potential new solar systems. Typical sensitivities to be reached will be ~10 mK, but deeper signal-averaging can be conducted if necessary. It should be noted that signal strength is not a limiting issue. Measurements at the

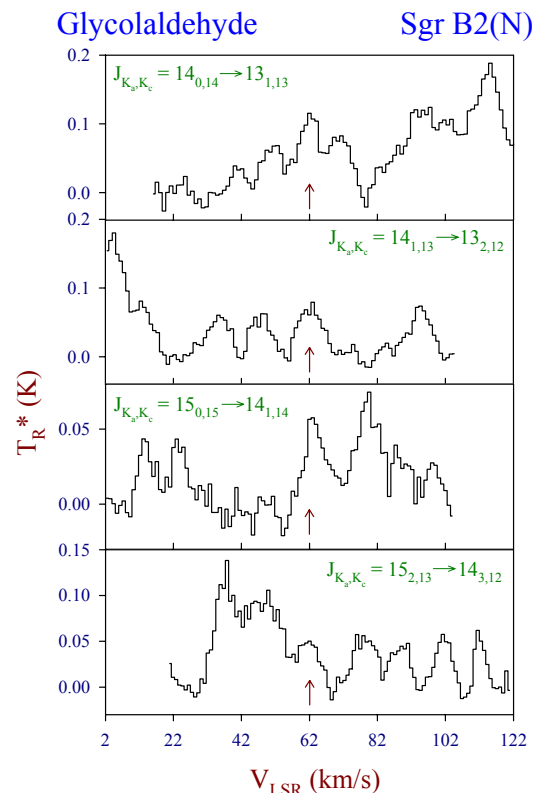


Figure 1.12. Some observed rotational transitions of Glycolaldehyde measured towards Sgr B2(N), the Galactic center molecular cloud, using the ARO 12 m telescope.

KP12m telescope have been conducted for as long as 130 hours of signal-averaging, to achieve levels of $T_{\text{rms}} \sim 0.0005$ K. More damaging will be contamination from other spectral features. However, given sufficient frequency coverage, enough rotational transitions can be studied to be certain about a given molecular identification.

1.8 Computational Modeling of Elemental Reactions Leading to Interstellar Ribose

The material falling from the interstellar space on Earth is a rich source of organic molecules. Recent assessments indicate that very significant quantities of organic material from meteoritic and cometary sources have been deposited on the primitive Earth (approximately $20\text{g}/\text{cm}^2$; e.g. Anders 1989) Seventeen amino acids, in every way identical to those made in the course of the famous Miller experiment, have been identified in the Murchison meteorite, which fell on Australia in 1969 (Chyba *et al.* 1990). It is estimated that more than 100 tons of meteoritic material fall on our planet each year; at the time of formation of the Earth, the bombardment was 10,000 times more intense. Thus, meteorites have brought an enormous quantity of organic molecules to Earth (Maurette *et al.* 1987).

The origin of chirality of living molecules (e.g. the exclusive involvement of D-ribose) is at present not satisfactorily explained. Engel and Macko (1997) have demonstrated that the Murchison meteorite contains an enantiomeric excess of certain L-amino acids that are today almost exclusively present in living systems. This result suggests that an extraterrestrial source for the excess enantiomers in the Solar System may predate the origin of life on Earth (Cronin & Pizzarello 1997). This excess may have resulted from the alteration of initially abiotic racemic mixtures by a process such as preferential decomposition from exposure to circularly polarized light (e.g. Bonner, Micura & Eschenmöser 1997).

Several difficulties were encountered in the synthesis of all pieces of an RNA molecule under primitive conditions (Joyce 1989). When one tries to produce ribose from formaldehyde and glycolaldehyde in the presence of sodium hydroxide and calcium acetate, by so-called "formose reaction", a very complex mixture is obtained, in which ribose is only a very minor component. Moreover, ribose is unstable on a geological time scale (Larralde, Robertson & Miller 1995). However, pentose and hexose phosphates can be obtained in good yields from glycolaldehyde phosphate when the reaction is run in the presence of formaldehyde (Müller *et al.* 1990). The outstanding problem at present is related to the synthesis of ribose with the exclusion of other aldopentoses (Zubay & Mui 2001).

The computational modeling will be one of the core activities in this project and will complement the experimental effort. The combination of astrophysical observations, laboratory and theoretical studies is needed to understand the complexity of the physico-chemical phenomena that occur in space. These are essential for testing and improving the existing astrophysical models and for the identification of molecules by laboratory studies and by observation.

Although much is known about the chemistry of dense interstellar clouds, much also remains uncertain, as a result of the variety of heterogeneous processes which may be important, including the effects of radiation fields and cosmic rays. Such conditions may vary significantly among and within different environments. Thus, the additional constraints on models supplied by

the identification of new molecular species and the determination of their abundance remains very important. Astrobiological studies that address the origin, evolution and distribution of life in the Galaxy require a fundamental understanding of the chemical processes and cycles that lead to organic chemistry in molecular clouds. Molecular clouds provide the initial organic inventory available to protostellar disks, and they can be the source of volatile organic material for the development of organic complexity of biogenic material. Energetic processes, such as irradiation and thermal processing may further increase the complexity of organics, as evidenced by laboratory studies. In this context the development of theoretical models of molecular synthesis and chemical pathways that can occur in the interstellar media in combination with laboratory data provide a basis to understand how molecular chemistry develops in interstellar material at different evolutionary stages.

The objective of this work will be to develop and implement multilevel modeling and simulation capabilities for understanding the elemental chemical reactions that may lead to formation of sugars (ribose) in the interstellar medium under various conditions. In particular, we will study the elemental processes involved in the formose reaction including its ion-molecule analog. The issues that will be considered in relation to the production of ribose in the formose reaction are: (i) the product selectivity under various conditions that can occur in the interstellar clouds, and (ii) the efficiency of the benzoin type condensation and the aldol condensations.

The Adamowicz research group has experience in developing methods in the area of molecular modeling, molecular quantum mechanics and molecular dynamics simulations. They have also used these methods to study chemical and physical properties of atomic and molecular systems relevant to interstellar chemistry (e.g. Lee & Adamowicz 2001). These include a series of studies concerning gas-phase amino acids performed with the use of molecular quantum mechanical methods and IR matrix-isolation spectroscopy (e.g. Stepanian *et al.* 1999, 2001). The effort in this project will focus on multilevel simulations of bi-molecular chemical reactions that can occur under various conditions (temperature, pressure, density, irradiation exposure, etc.) in space and leading towards synthesis of sugars.

In the simulation work performed with the use of quantum modeling and quantum mechanics interfaced with molecular dynamics, we will develop static and dynamic models enabling simulation of reaction cycles involving elementary molecular precursors and leading to synthesis of sugars. The simulation methodology will be implemented on a massive parallel processing system (MPPS) using novel computational architectures. The models will serve as a roadmap towards developing a fundamental scientific understanding of the investigated molecular systems and their interactions occurring under conditions that may involve high collisional velocities and intense irradiation.

1.9 Tracing Abundances of Organic Molecules from Clouds to Protoplanetary Disks

Complex molecules are produced in a variety of environments, including the inner envelopes (and possibly the outer envelopes) of carbon-rich AGB stars as well as the cores of dense interstellar clouds. As of the present, very little research has gone into the subject of how these molecules are formed, except for two specific classes of species. The production of PAH's (polycyclic aromatic hydrocarbons), ranging in size from species with perhaps 30 carbon atoms to much larger objects, has been considered in warm inner regions surrounding AGB stars. The

basic idea is that under appropriate conditions, the large amount of acetylene present can be partially converted into simple aromatic species such as benzene and naphthalene. These molecules can then grow into much larger PAH's via a high-temperature radical-based synthesis akin to the production of soot via combustion of petroleum in terrestrial laboratories and automobiles (Frenklach & Feigelson 1989). The production of fullerenes (C₆₀, etc.) has been studied in the more rarefied and oxygen-rich atmospheres of interstellar clouds, where a detailed scheme involving low-temperature ion-molecule reactions has been proposed (Bettens & Herbst 1995, 1996, 1997) based on the laboratory work of Bowers and co-workers (von Helden *et al.* 1993), in which fullerene production proceeds through the initial production of straight-chain carbon clusters, followed by large single-ring and double-ring systems. The production of large clusters of carbon atoms, of unspecified structure, has been considered in supernova remnants by Clayton *et al.* (1999) who extended the methods of Bettens & Herbst (1995, 1996, 1997) to form actual carbonaceous grains.

1.9.1 Molecular Cloud Chemistry:

The gas-phase formation of PAH's under interstellar conditions is not likely unless the PAH's are hydrogen-poor because it is difficult for gas-phase processes to hydrogenate large molecules at low temperature (Bettens & Herbst 1995). This constraint is important for the production of other classes of organic molecules. Most of the larger ones found in typical dense interstellar clouds are exceedingly unsaturated, with species such as C_nH radicals and the polyynes (HC_nN) important. Indeed, what relatively hydrogen-rich species exist unambiguously in space are found in local regions of dense interstellar clouds near sites of high-mass star formation. These sources, known as hot cores, are typically much warmer than the ambient dense interstellar medium (100-300 K rather than 10-30 K). Hydrogenation is thought to occur not in the gas, but on the surfaces of dust particles in a prior and cooler stage, where it is brought about by fast-diffusing hydrogen atoms. The observations of hydrogen-rich, or "saturated," molecules in the gas phase in hot cores is thought to signify that molecules on the mantles of dust particles have been released into the gas owing to the rise in temperature. The largest molecules detected in such hot cores are simple ethers (dimethyl ether, and possibly ethyl methyl ether and diethyl ether - see Charnley *et al.* 2001), alcohols (methanol and ethanol), acetone, and methyl formate. Intensive searches in the past for glycine have only achieved ambiguous results. Larger molecules than these, including biogenic species, are certainly present in hot cores, since the abundances of these smaller organic species are often quite high. But, progress awaits the measurement and analysis of the spectra of larger species in the laboratory.

To understand the abundance and distribution of complex molecules (defined roughly as organic species with greater than 10-15 atoms) throughout the interstellar medium, we propose to enlarge our current chemical model networks to include both the formation and destruction of a wide variety of such species. Although a few studies of the actual rate of destruction of complex molecules via both chemical reactions and photons have been published, on balance little is known about complex molecular lifetimes in assorted regions of interstellar space. In the absence of detailed information on the rates of formation and depletion, we will use a variety of theoretical methods, principally statistical theories of reaction rates, as detailed by Bettens & Herbst (1995) in their fullerene analysis. Such methods have indicated that large molecules become quite stable against photodissociation and can even exist for long periods in relatively unshielded diffuse interstellar clouds. We currently have three networks that already have some

complex species in them: (i) a model for the gas-phase chemistry that occurs in the carbon-rich, low-density outer envelopes of AGB stars and protoplanetary nebulae (Millar *et al.* 2000; Woods *et al.* 2003), which currently contains a small number of species through 25 carbon atoms in size, (ii) the model for fullerene production in the interstellar medium (Bettens & Herbst 1997; Ruffle *et al.* 1999), which also contains the chemistry of other types of very unsaturated hydrocarbons, and (iii) a model for hot-core chemistry that contains both gas-phase and surface chemistry (Caselli *et al.* 1993). These model networks will be extended to include larger varieties of complex species, especially molecules, such as the simple amino acids and heterocyclic rings, important in the context of pre-biotic synthesis. A suggested interstellar synthesis of glycine and other amino acids has recently been published (Blagojevic *et al.* 2003).

It is likely that the more saturated alcohols, esters, and ethers will be produced efficiently in star formation regions, where dust chemistry is important (Charnley *et al.* 2001). Until quite recently, models of the chemistry occurring on dust particles have suffered from a basic problem: typical rate equations are not adequate to explain what happens when only a small number of reactive species are present on a given grain at any time. A new method, known as the direct master equation approach (Green *et al.* 2001, Biham *et al.* 2001) has now been adapted by us (Stantcheva *et al.* 2002; Stantcheva & Herbst 2003) and should be able to solve the surface chemistry problem exactly if the correct surface reactions are delineated and their rates understood. The actual chemistry of star formation regions such as hot cores involves a close interplay between gas and dust. Molecules such as methanol, produced mainly on grains, can desorb into the gas and be the precursors for more complex species formed via gas-phase reactions. We are currently collaborating with a group of Norwegian and Canadian chemists to measure some of the gas-phase reactions that have been suggested.

1.9.2 Complex molecules in protoplanetary disks:

The protoplanetary disk stage of stellar evolution, in which a young, low mass star known as a T Tauri star, is at the center of a dense, optically thick disk of gas and dust, is of extreme interest because these disks are the precursors to planetary systems. Observations of gas-phase molecules by radio astronomers show that the fractional abundances of heavy species such as CO and HCN are significantly lower than in dense interstellar clouds (Dutrey *et al.* 1997). The obvious interpretation, that many of these molecules have been accreted onto dust particles in disks, appears to be the right one. In fact, current models of the chemistry occurring in protoplanetary disks (Aikawa *et al.* 2002; Willacy & Langer 2000) show that at distances greater than ~ 50 AU from the star, all molecules heavier than H_2 in the midplane of the disks should condense out in far less time than the typical million-year-lifetime of a T Tauri star/disk system. But disks are not flat despite their name; they are known to flare out with increasing distance from the star, so that there is a coordinate for height (Z) as well as a radial coordinate. At very large heights, gas-phase molecules tend not to be present in current models, mainly because the molecules are photodissociated by relatively unimpeded UV radiation and X-rays, both from the central star and from the interstellar medium. Sizeable abundances of gas-phase molecules exist, however, mainly in regions of intermediate height, where the temperature is warm enough to evaporate the molecules from grain surfaces after they accrete onto them, and the radiation field is not intense.

The current state of chemical models of protoplanetary disks is as follows. Models that follow the chemistry of disks with both a vertical and a radial structure are static in nature; that is, the physical conditions, though strongly heterogeneous, are assumed to be constant (Willacy & Langer 2002; Aikawa *et al.* 2002). In these models, sedimentation and coagulation are not included although they are clearly of great importance for planetary formation. Models that include some dynamics do not include the vertical coordinate; i.e., they are one-dimensional models of the midplane. In these models, chemistry occurs during the inside-out collapse from a dense interstellar core and continues to occur as parcels of gas move inwards towards the central star under steady accretion due to angular momentum loss via viscosity (Aikawa & Herbst 1999). The material becomes almost totally solid-state in nature except for molecular hydrogen but can evaporate from the dust particles once the distance to the star becomes sufficiently short. No model that we are aware of contains complex molecules, although it is vital to follow their fate in a protoplanetary disk.

We propose to remove the current shortfalls of one-dimensional and two-dimensional chemical models. First, we will include complex molecules in them. The complex molecules will have initial abundances produced in our dense cloud models. But, since grain chemistry will be active, and since temperatures will rise near the T Tauri star, it is likely that we will form more complex molecules in processes similar to those occurring in hot cores. We will focus initially on one-dimensional models because the accretion of large molecules onto dust particles is clearly important for astrobiology. In addition to both gas-phase and surface chemistry, processes to be considered include coagulation of small dust particles into larger objects, accretion shocks, and inward radial motions. To determine photodestruction rates of complex molecules, we will utilize statistical theories (Bettens & Herbst 1995). Once one-dimensional models have been successfully upgraded, we will turn to our two-dimensional models. One specific question of interest is the height of the zone in which molecules are depleted from the gaseous state. This height would certainly be related to the planarity or lack thereof of the planetary system that is produced.

1.10 Role of Membranes in the Evolution of Cellular Life

Clearly the presence of the molecules of life is a necessary prerequisite; yet it is also necessary for them to be confined to surfaces or contained within a suitable compartment within which the formation of macromolecules may be possible. In either case, the effective concentration is increased and can promote further reactions, which would be improbable in the gas phase. The formation of membranes involves amphiphilic compounds, which in aqueous solution are known as surfactants (detergents) and biological lipids.

Biological membranes mediate many of the distinctive functions of life on earth, and their formation is prerequisite to any conceivable form of cellular life. It is known that membranes comprise a lipid bilayer, which provides a permeability barrier to the passage of ions and polar molecules, together with proteins which mediate various biological functions, including active transport, photoreception, light energy transduction, and the generation of electrical signals. At the present time two generic schemes for the origin of cellular life on earth are under discussion. The first supposes initially that small molecules were formed within a primordial aqueous environment, leading eventually to their polymerization and subsequent incorporation within a membrane-encapsulated volume to yield the earliest cells. In the second scheme, spontaneous

self-assembly of amphiphiles into bilayer vesicles preceded polymerization of small molecules, with further membrane growth occurring by a photosynthetic process. Moreover, a further consequence of this compartmentalization is that gradients of chemical potentials of various solute species present in the prebiotic aqueous environment would be possible, e.g. as a consequence of photosynthetically produced gradients of H^+ or other ions. Thus a source of free energy for polymerization systems involving small molecules would exist, e.g. involving nucleotides or activated amino acids.

The latter mechanism is plausible since common amphiphiles can be formed from relatively simple precursors such as long chain alcohols and inorganic phosphate (Chachaty *et al.* 1988; Caniparoli *et al.* 1988). Such organic amphiphiles are found in carbonaceous meteorites (Deamer 1985; Deamer & Pashley 1989). The proposed studies will focus upon the investigation of dialkyl phosphates as plausible models for prebiotic amphiphiles. These compounds exhibit sufficient richness of polymorphic phase behavior that they are able, depending on the environment, to form a variety of self assembled structures.

The specific objectives of the proposed work will encompass the following:

- 1) Determination of phases diagrams for aqueous dispersions of a homologous series of dialkyl phosphates, in which the number of chain carbons $n = 6, 10, 14, 18$;
- 2) Characterization of influences of salt and pH on temperature-dependent polymorphism of aqueous dispersions of dialkyl phosphates;
- 3) Characterization of isotropic micelles and lamellar and reversed hexagonal phases of dialkyl phosphates; investigations of conditions necessary for spontaneous vesicle formation;
- 4) Comparative studies of average properties of dialkyl phosphates in different organized assemblies by deuterium (2H) NMR lineshape analysis (Brown 1996); investigation of dynamical properties at the molecular level by nuclear spin relaxation measurements (Martinez *et al.* 2002).

Very briefly, modern state-of-the-art nuclear magnetic resonance (NMR) methods will be applied to investigate the average thermodynamic properties and phase behavior of organized assemblies of dialkyl phosphates in water (Brown & Chan 1996). These and related amphiphilic compounds have been hypothesized to be implicated in early protobiological assemblies leading to encapsulated membrane systems, self replication by photosynthetic growth, polymerization of small molecules, and eventually life on earth as we know it. The polymorphic phase behavior of a series of dialkyl phosphates will be investigated as a function of variables to include temperature, salt, and pH. These studies will provide knowledge of the requirements for formation of highly curved surfaces, leading to the formation of closed membranous structures such as vesicles. We will test the hypothesis that the curvature free energy of the membranous assemblies is a crucial variable leading to the formation of closed membrane vesicles. In addition the microscopic configurational and dynamical behavior of the lipid systems will be investigated (Nevzorov, Trouard & Brown 1998). The latter will establish a connection between microscopic properties and bulk or average properties of the systems, which may be important both with regard to the polymorphism of the assemblies, as well as the interaction of the amphiphiles with other lipid constituents such as polyisoprenoids, which may represent chromophores, found in the prebiotic milieu.

2.0 Module 2: Formation and Evolution of Habitable Worlds

Team: L. Close, M. Giampapa, A. Glassgold, P. Hinz, D. Kring, J. Lunine, R. Malhotra, M. Meyer, J. Najita (Deputy), and S. Strom (Lead).

2.1 Introduction

Gas giant planets are the most readily observable diagnostic signatures of emerging and mature planetary systems. They play a decisive role in determining whether earth-like planets can form and survive in habitable zones. They sculpt the remnant debris disk of planetesimals, they control, both the influx of volatiles delivered to terrestrial planets in the inner solar system as well as the rate of giant impacts over geologic time. Our proposed program provides measurements which directly constrain when giant planets form, and where they are located in mature planetary systems—observations central to understanding the likelihood that life-bearing planets can form, survive, develop oceans and atmospheres, and sustain biological trends for long periods absent cataclysmic events.

We make use of ground- and space-based spectroscopic observations mapping the gas content of disks surrounding stars of differing ages to determine how long gas sufficient to form giant planets is present. The existence and location of giant planets can then be inferred from spectroscopic signatures of “tidal gaps”.

In addition, we make use of ground- and space-based infrared and submillimeter emission arising from small dust grains in circumstellar disks with ages from 3 Myr to 3 Gyr—from when planets are forming to when planetary systems are mature. Spectral energy distributions and low-resolution spectra probe the total dust mass as well as its radial distribution and composition. In combination with theoretical models, these observations provide the basis for inferring the location of giant planets, planetesimal collision rates in exo-terrestrial planet zones and the rate at which volatiles are transported from the outer to inner solar system.

The proposed efforts thus speaks directly to road map goal 1, and provides data which serves as context for the design and science strategy of a TPF mission, goal 1.2.

The third part of the module provides essential constraints on the development of atmospheres and climatic variations through observations of variability and activity among sun-like stars, spanning ages from the earliest phases of accretion activity to characterization of the range of variations for sun-like stars throughout their lives.

In the pre-main sequence phase (1-30 Myr), large variations in the x-ray and UV flux could play a significant role in ionizing the circumstellar disk and driving chemistry important for determining abundances of organic molecules. Indeed the results from this study will be important for the work described in Module 1, as well as the modeling of observational results on gas-rich disks in this module.

Over longer timescales, we will characterize the mean and dispersion in solar flux by observing sun-like stars from 30 Myr to the age of the Sun. The sensitivity of earth’s climate to modest

variations in insolation is well known. The Maunder sunspot minimum is associated with a severe cooling of the Northern Hemisphere, and associated famine. Here we are both interested in how solar cycle variability has changed with time, and how it can be expected to change in the future. The decline in stellar activity with age is well known, and here we focus on a quantified analysis not only of general trends, but of excursions about the average. The Sun is apparently much less variable than typical stars of its age, and far less variable than younger stars. Is the Sun's relative stability responsible for providing a hospitable evolutionary environment on earth? If so, how frequently do solar-type stars exhibit such benign activity excursions?

These measurements provide crucial connection between studies of complex organic chemistry in circumstellar disks (Module 1) to investigations of climate variability such as those undertaken by the NAI focus group "Mission to Early Earth" addressing NAI Roadmap Goals 4.1 and 6.1.

2.2 Task A: Gas Rich Disks

2.2.1 Overview

Understanding the formation of giant planets is critical to understanding the origin of the Earth and the potential for habitable extra-solar planets. On the one hand, Wetherill has suggested that the development of life on the Earth may be a consequence of the existence of Jupiter, because Jupiter probably cleared the inner solar system of planetesimals that would otherwise have impacted the Earth at a damagingly high rate. On the other hand, at earlier times, giant planets may have worked *against* the survival of earth-like planets. For example, the discovery of extra-solar giant planets at small orbital radii (~ 0.1 AU; e.g., Marcy and Butler 1998) suggests that giant planets migrate readily inward from their formation distances at larger radii (~ 5 AU; e.g., Boss 1995). Giant planets that form early, e.g., during the disk accretion phase in which orbital migration is likely to be rapid, are likely to migrate in close to their stars, sweeping along any earth-like planets that have already formed at smaller radii. Solar systems in which giant planets form late, at the end of the disk accretion phase, have the best chance of preserving earth-like planets at AU distances (e.g., Trilling *et al.* 1998). These considerations raise fundamental questions regarding the origin of planetary systems: where and when do giant planets form?

Where do Giant Planets Form? Traditionally, theories of giant planet formation have focused on the growth of planets under the protoplanetary disk conditions expected at ~ 5 AU. However, the large spread in the orbital radii of the known extra-solar planets may indicate that giant planets actually form over a range of disk radii and physical conditions. Indeed, it is probably inaccurate to assume that planets formed where they are now observed to be because dynamical effects, such as orbital migration due to tidal interactions between the disk and protoplanet and dynamical scattering between planets following disk dissipation (e.g., Lin and Ida 1997), are likely to significantly alter planetary systems. In order to determine the formation distances of planets, we need to carry out a census of young (1 – 10 Myr) planetary systems. Ideally, we would hope to measure the masses and orbital radii of planetary companions, for comparison with the properties of older (several Gyr old) systems, in order to begin to chart out the evolution of planetary systems.

When do Giant Planets Form? What is the likelihood that disks that have ceased accreting (at ages $t > 1$ Myr) still have the gas reservoirs needed to form giant planets? Moreover, is the

actual gas dissipation timescale consistent with present theories of giant planet formation? Current theory requires that the gas in disks survive for ~ 10 Myr in order for planetary cores to accrete a massive gaseous envelope (e.g., Podolak *et al.* 1993). However, existing studies of the gas in outer disks (>50 AU; e.g., Zuckerman *et al.* 1995), indicate a giant planet formation timescale <10 Myr. Additional evidence for the rapid dissipation of disks comes from studies of the IR excesses of young stars, which show that inner disks ($r < 1$ AU) become optically thin in concert with the cessation of stellar accretion, i.e., on timescales <10 Myr (e.g., Strom *et al.* 1989). These results favor the *early formation* of giant planets which is less advantageous for the survival of Earth-like planets. Moreover, these results, combined with the now frequent detection of extra-solar planets via radial velocity techniques, suggest that giant planet formation theory may require serious revision. Unfortunately, the observational motivation for a theoretical overhaul is far from definitive because there have been no direct measurements of the gas content of disks within ~ 5 AU. We propose to test this scenario by measuring the gas dissipation timescale in disks at radii < 5 AU. If we find that abundant reservoirs of gas persist beyond the stellar accretion phase, we will establish the possibility of an extended period of giant planet formation and the likely preservation of earth-like planets. The proposed study will also place a fundamental constraint on theories of giant planet formation. Finally, the spectroscopic diagnostics that we propose to develop will lay the groundwork for future opportunities: the indirect detection of forming protoplanets and the measurement of planet formation distances (see Section 2.3).

2.2.2 Proposed Program

Observational: We will search for molecular emission from disks at <5 AU surrounding nearby (< 150 pc) sun-like stars in the age range 1-10 Myr. Since the angular scales involved are much beyond our current capability to resolve spatially (1 AU at the nearest star forming regions at 150pc is <10 milli-arcseconds), we will use high-resolution spectroscopy to determine where in the disk the detected gas resides. The detected emission strengths will be converted into gas content as a function of disk radius using the results of the theoretical studies described below. Diagnostics in the thermal infrared (4-30 μ m) are ideal for this study since the Planck function for disk material at < 5 AU peaks in the mid-infrared. At the warm temperatures (100 – 2000 K) and high densities of disks at these radii, molecules are expected to be abundant in the gas phase, and sufficiently excited to produce a rich ro-vibrational and rotational spectrum. We are part of a team that will utilize modest resolution ($R=600$) spectra to be obtained with SIRTf through the Legacy Science Program (Meyer *et al.*) to constrain the lifetime of gas-rich disks capable of forming gas giant planets. Abundant molecules such as CO, OH, H₂O, and H₂ have transitions in the mid-infrared, and can be used to trace the structure and dynamics of disks. Work to date on high-resolution IR spectroscopy of disks has shown that the CO overtone (2.3 μ m), CO fundamental (4.6 μ m), and H₂O ($\sim 2\mu$ m) ro-vibrational lines can be used to probe the kinematics and physical structure of disks at radii < 2 AU (Fig. 2.1; see also Najita *et al.* 1996, 2000, 2003), i.e., in what is today the terrestrial planet region of the solar system. By extending these studies to other molecular species and wavelengths (e.g., OH, H₂ and longer wavelength H₂O lines), it should be possible to extend these studies to the larger distances traditionally considered in giant planet formation theories ($r > 5$ AU). We plan a two-pronged approach which includes: 1) complete pilot survey using high resolution near-IR spectroscopy to survey nearby young stars; and 2) utilize ground-based mid-IR echelle spectrometers to follow-up objects detected in the SIRTf Legacy Science Program of Meyer *et al.* (described below).

Theoretical: The observations will be complemented by a detailed theoretical study of the thermal and chemical structure of gaseous inner disk atmospheres. Disk atmosphere calculations to date refer primarily to the temperature structure in the dust component of the disk (e.g., D'Alessio *et al.* 1998; Chiang and Goldreich 1997). However, the gas and dust components are poorly coupled thermally in the upper disk atmosphere. Consequently, the temperature structure of the gaseous atmosphere requires its own calculation. For the proposed program, we will build a detailed study of the thermal and chemical structure of disk atmospheres that includes all of the diagnostics to be studied observationally.

2.2.3 Future Opportunities

The spectroscopic diagnostics that we have proposed to develop will also lay the ground-work for future opportunities: the indirect detection of forming protoplanets and the measurement of planet formation distances. We will develop this potential technique to the extent possible during the proposed funding period.

Indirect Detection of Forming Protoplanets: It may be difficult to detect young planets directly during the epoch of their formation (i.e., when a substantial circumstellar disk is still present): the much larger emitting area of the disk compared to the planet may make it difficult to detect the planet in the glare of the disk. Thus, we may have to rely on a more indirect, dynamical signature of the presence of planetary companions. Dynamical theory predicts that as a giant planet forms, tidal interactions between the planet and disk clear a region in the disk, a "gap", within which the planet orbits (Lin and Papaloizou 1993; Takeuchi *et al.* 1996). Since the width of the gap depends on planetary mass, measurements of the location and width of gaps in protoplanetary disks can ultimately provide us with a method of inferring both the masses and orbital radii of planets at their epoch of formation. Given the small angular scales subtended by inner disks (and the even smaller angular width of gaps created by giant planets) e.g., Jupiter-mass companions will produce ~ 0.3 AU wide gaps at an orbital distance of 1 AU; Takeuchi *et al.* 1996). The most promising approach by which it would be possible to search for forming giant planets in the next ~ 5 years is through high resolution spectroscopy. With this technique, we would search for line emission from the gap which will appear bright against the absent continuum emission from the gap. High spectral resolution will be used in lieu of high angular resolution to identify the range of disk radii over which the gap extends. The resulting spectral energy distribution (SED) will be indistinguishable from that of a disk without a gap. Even with the high photometric accuracy and continuous wavelength coverage of SIRTf (or JWST) observations of disks in the mid-infrared, such small gaps will be impossible to detect given the ambiguities involved in interpreting SEDs. Our simulations indicate that 8-10m telescopes have the sensitivity to detect spectroscopically gaps created by Jupiter-mass companions in the nearest star-forming regions.

Infrared Diagnostics of Protoplanetary Disks

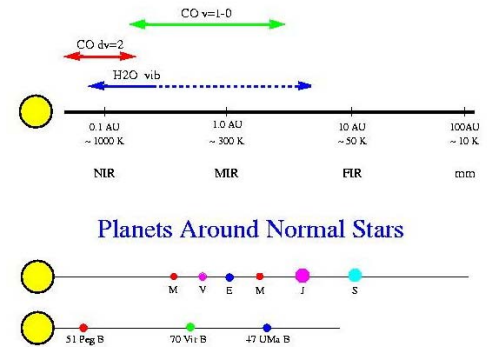


Figure 2.1 Infrared spectral line diagnostics of disk: The CO overtone ($\Delta v=2$, $2.3\mu\text{m}$), CO fundamental ($v=1-0$, $4.6\mu\text{m}$), and the ro-vibrational water lines (K-band), probe the structure of disks.

2.3 Task B: Evolution of Planetary Systems

2.3.1 Overview of Debris disks

The growth and survival of earth-like planets depends critically on the architecture of the parent planetary system: Jovian mass planets in or near the terrestrial zone will doom the formation of earth-like planets (Jones, Sleep, & Chambers 2001), but may have life bearing satellites of their own. The likelihood that planets in the terrestrial zone will have oceans and life-friendly atmospheres may well depend on this architecture as well, since transport of volatiles from the outer solar system is believed linked intimately with the relative location of the terrestrial planets, giant planets and outlying cometary material. Finally, whether life on an earth-like planet has sufficient time to evolve—even on apparently hospitable worlds—depends on the number and time between cataclysmic collisions of the sort that resulted in the extinction of the dinosaurs. The collision frequency in turn is linked to the architecture of the parent planetary system: ‘favorably’ located giant planets can quickly remove planetesimals from the terrestrial zone, while earths in systems with distant Jupiters or none at all may suffer high, potentially life-stultifying collision rates.

The Space Infrared Telescope Facility (SIRTF) is a cryogenically cooled mid- to far-infrared space telescope with unprecedented sensitivity to be launched by NASA this spring. The University of Arizona and NOAO are heavily involved with this mission, contributing one of the scientific instruments and leading two of the major data collection (“Legacy”) projects. This expertise and the data will be made available to the NAI as part of the Arizona membership. With the advent of the SIRTF satellite, we can for the first time carry out observations diagnostic of (i) planetary architectures, and (ii) the rate of collisions among large bodies in terrestrial zones for a large number of sun-like stars. These span a wide range of ages—from 1 Myr to 5 Gyr, equivalent to pre-Hadean to the present. These observations, combined with dynamical modeling of simulated exo-solar systems can provide the basis for placing our solar system in context. We can assess the likelihood that habitable planets exist and the potential for life’s surviving and evolving on those planets.

We plan to use precise infrared spectral energy distributions from SIRTF to infer the surface density, temperature and approximate mineralogy distributions of small grains surrounding sunlike stars. Ground-based imaging both of light scattered earthward by the dust, and of thermal emission from dust grains provide incontrovertible evidence that this dust is arrayed in a disk of dimension several hundred astronomical units.

The lifetime of dust grains with sizes of order 1 micron (typical of those responsible for producing both thermal emission and scattered light) is well less than 1 Myr—the time required for Poynting-Robertson drag to cause such grains to spiral inward toward the surface of the parent star. The dust disks are thus “second generation” material—dust released

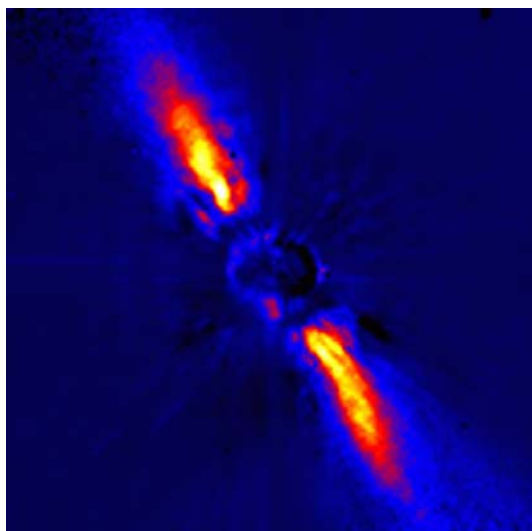


Figure 2.2: Adaptive optics image of light scattered earthward by the dust disk surrounding the nearby star, β Pictoris (ESO NTT). The light of the central star has been occulted by a coronagraphic disk.

from larger parent bodies such as asteroids or comets through fragmenting collisions or sublimation. Further, the presence of large, planetary masses is *required* in order to stir the smaller planetesimals; planetesimals alone are not capable of sufficient mutual perturbation.

Recent images of nearby debris disk systems show that some disks possess central gaps comparable to the orbit of Neptune in our solar system, as had been inferred previously based on the observed spectral energy distribution shape (Fig. 2.3).

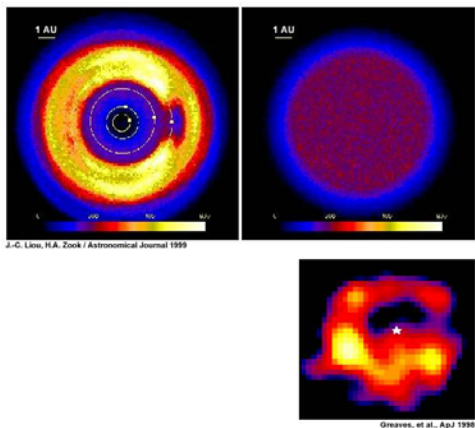


Figure 2.3. A comparison of thermal emission from the dust disk surrounding the star Epsilon Eridani (lower right; Greaves et al. ApJ, 1998) with two computer simulation (Liou & Zook 1999) of how our solar system (upper left) would look to an outside observer; four dots represent Jupiter, Saturn, Uranus and Neptune. Blue represents a relative ‘dust void’ (resulting from dynamical ejection of colliding bodies from the inner solar system by Jupiter). By contrast, note the even distribution of dust throughout the model solar system having no giant planets (upper right). Epsilon Eridani appears to have an “inner hole” analogous to that found in our own solar system.

The significance of debris disks is that they offer surprisingly easy means for inferring the existence of planetesimals and/or planetary systems. They can be inferred from infrared excesses arising from secondary grains arising from collisions. Their architecture can be inferred both from the shape of spectral energy distributions and from subsequent resolved observations with large, ground-based telescopes (Li & Lunine 2003), and their evolution can be traced from observations of large samples of sun-like stars spanning a wide range of age.

From study of the radial distribution of our own solar system dust, for example, one could infer not only the existence of the asteroid belt and Kuiper Belt, but also the presence of planets with locations and masses, e.g. that the planetesimal populations are dynamically “hot”.

2.3.2 Proposed Programs

Observational: UA astronomer and proposal deputy PI Michael Meyer and colleagues from Arizona, Caltech and elsewhere have been granted observing time, as a coherent (“Legacy”) program, to observe 345 solar-like stars ranging in age from 3 Myr to 3 Gyr with SIRTf. The goals of this program are to use precise spectral energy distributions (from 3 microns to 160 microns) to (i) constrain the structure and composition of disks; (ii) trace the evolution of gas and dust disk structure and mass over time; (iii) infer the presence of planets at orbital radii ranging from 0.3 to 30 AU. These observations form the basis for addressing several questions key to the planet formation part of the astrobiology roadmap (Goal 1).

Building on the planned SIRTf program (Meyer *et al.* 2001), we will carry-out follow-up surveys with state-of-the-state ground-based platforms aimed at providing spatial information, crucial for breaking potential degeneracies inherent in modeling spectral energy distributions. Meyer, Close, and Hinz will utilize the high resolution MMT-AO system with the ARIES and MIRAC/BLINC cameras (see Module 3 for technical detection) in direct imaging mode to provide the needed observations for our strongest SIRTf detections (~10-30 stars). A similar

capability is planned for the Magellan telescope in the southern hemisphere within the period of performance of this proposal. We also plan follow-up studies at high spatial and spectral resolution with the IRIS (medium resolution mid-IR spectrograph for use with the MMT and Magellan) to look for evolution in dust mineralogy across resolved circumstellar disks. For a similar-sized sample of candidates with weak disk emission, we will utilize the LBTI instrument described in Module 3 to search for remnant dust that could complicate the detection of earth-like planets with TPF (Roadmap Goal 1.2).

Theoretical: Under the proposed NAI membership, Malhotra, Lunine, Kring, and colleagues will develop models constrained by the SIRTf and ground-based data. Our ultimate goal is to connect observational studies of the evolution of planetary systems with the cratering record of our own solar system (under study by the proposed NAI Impacts Working Group) as a tool to understand the effects of solar system dynamics on the evolution of habitable zones.

Constraining collision rates in the terrestrial planet region: SIRTf observations will provide measures of dust optical depth as a function of distance from the parent star via observed excess infrared emission above photospheric levels (*near*-infrared, 10-20 micron, excess emission provides a measure of dust optical depth in the terrestrial planet region). Because the grain population in the disk is ‘secondary’, dust optical depth is directly related to collision rates between planetesimal-sized bodies. By comparing observed dust optical depths in terrestrial planet zones for sun-like stars of differing age in our SIRTf Legacy sample with those at differing epochs of our own solar system (derived from observations of the Zodiacal Cloud and inferred from cratering histories) we can determine whether collision rates for exo-solar systems are higher or lower than our own. If the typical rates inferred for exo-systems are higher, the frequency of devastating impacts on earth-like planets will likely be higher—diminishing the likelihood that advanced life forms develop.

Presence of interesting organic materials in disks: University of Arizona Theoretical Astrophysics postdoctoral fellow Aigen Li and Lunine have demonstrated with UKIRT (United Kingdom Infrared Telescope Facility) the ability to distinguish the presence or absence of PAH’s in disks that are remnants of planet formation around nearby stars (Li and Lunine, 2003; Li and Lunine, in prep). The presence or absence of PAH’s seems to be tied to the variation in geometry and hence conditions from one disk to another, and should provide insights into the distribution of organic material present in such disks. The results of these studies for SIRTf-detected disks will be as a boundary condition for the modeling of the distribution and delivery of organics to terrestrial planets based on dynamical models Lunine has pursued with colleagues in Europe (Morbidelli *et al.* 2000) and the University of Washington (Raymond, Quinn, & Lunine 2003). It will also be an input into the chemical studies of complex molecule formation in protoplanetary environments (Module 1).

Planetary System Architecture: Observed spectral energy distributions will provide estimates of the surface density of micron-size dust as a function of distance from the parent star, $\Sigma(r)$ (Li & Lunine 2003). In turn, $\Sigma(r)$ provides the basis for inferring the number of collisions among planetesimals as a function of radius, a quantity that reflects the both the current and past dynamical history of the disk, and the role of giant planets in shaping that history. We plan to combine $\Sigma(r)$ distributions inferred from SIRTf Legacy observations with dynamical modeling

to infer (i) planetary architectures, and (ii) the rate of volatile transport from outer to inner solar system regions.

University of Arizona co-I Malhotra and collaborators will use the configurations of giant planets inferred from SIRTf observations to model the dynamical evolution of planetesimal swarms in these systems. We will employ N-body integrators developed by Malhotra (1996) and Hahn and Malhotra (1999) for the co-evolution of giant planets and planetesimal disks to predict $\Sigma(r)$ for different initial configurations of giant planets. These $\Sigma(r)$ predictions can then be compared with those derived from SIRTf observations, thus constraining plausible planetary architectures.

We will compute the probability that planetesimals starting at a given semi-major axis would collide with terrestrial planets on various stable orbital configurations in the habitable zone. For each initial semi-major axis at which planetesimals are initiated in the simulation, based on nebular models, we can associate a particular set of volatile abundances including water and organic compounds (Lunine, Owen, & Brown 2000). Thus we will track, in concert with the probability of collision with potentially habitable planets, the amount of ocean-forming and life-forming materials putative terrestrial planets will gain.

Computation of volatile load of planetesimals will be guided by the results for our own solar system. While detailed models of planetesimal composition do not uniquely define the composition of a planetesimal swarm versus semi-major axis, we are mostly interested in the existence of major volatile species such as water and organics, rather than details such as the chemical form of nitrogen (ammonia or molecular nitrogen) and such other issues. Water-bearing planetesimals include those with water ice or bound water of hydration, equivalent in our own solar system to the icy planetesimals of the outer solar system and of the asteroid belt. Organics can also be predicted based upon what is seen in the major meteorite types as well as what is contained in comets. We thus will label planetesimals “water-bearing” or not, and “organic-bearing” or not, with rough inventories based upon the cometary and asteroidal (meteoritic) analogs in our solar system. This will be sufficient to define the probability of volatile delivery to the habitable zone, as shown by Morbidelli et al (2000). Hence these calculations will serve as input for ongoing calculations by Lunine in collaboration with Sean Raymond and Tom Quinn at the University of Washington (Raymond, Quinn, & Lunine 2003) to predict the delivery of volatiles during large-body accretion associated with the terminal phases of terrestrial planet formation (Chambers & Cassen 2002). While these calculations have been ongoing in parallel using statistical distributions of giant planets, the SIRTf data will give us the first opportunity to use observations to determine locations of giant planets, and hence predict the dynamical environment and delivered volatile inventory to possible terrestrial planets in the habitable zones of those systems.

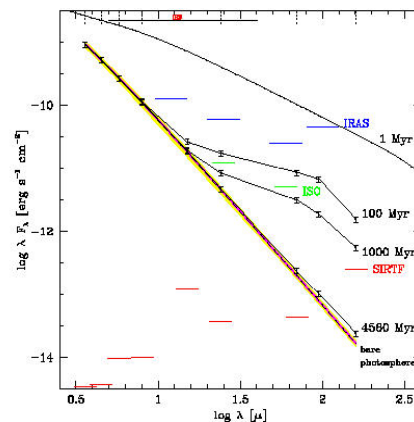


Figure 2.4: Model spectral energy distributions for a hypothetical solar system surrounding a solar-like star located at a distance of 30 pc, for ages 4560, 1000, and 100 Myr. Indicated in the figure are the limits of the IRAS survey, and the predicted limits of the Meyer et al. SIRTf Legacy survey observations.

2.4 Task C: Solar irradiance changes from formation onwards

The next stage of evolution of terrestrial planets after disk dispersal is evolution in the presence of stars that themselves evolve over time as they enter the main sequence phase of hydrogen burning. Stars like the Sun vary in energy output on a range of timescales. This module will, for the first time, systematically quantify such variations.

2.4.1 Overview

The changing output of solar-type stars (total, ultraviolet and x-ray luminosity)—from the time of planet-formation to the current epoch—is needed to understand: (i) the formation and early evolution of planetary atmospheres ($t < 500$ Myr); and (ii) climatic variations among more mature planets ($t > 500$ Gyr). Charting overall energy output and cyclic solar activity on sun-like stars spanning a range of ages thus provides crucial insight into how frequently earth-like atmospheres are likely to form and survive, and how frequently exo-earths encounter benign climatic variations.

The solar atmosphere exhibits a variety of magnetic field-related phenomena—powerful flares, cool spots, hot active regions, episodic mass ejections, the warm 10,000-degree chromosphere and the 2 million degree corona, and the sunspot cycle—that we refer to collectively as “activity”. The signature of the nonradiative heating in many of these magnetic active areas is easily detected by the enhanced radiation it produces in chromospheric spectral lines, such as the Ca II H and K resonance features near 400 nm. Similarly, evidence for this same kind of activity is readily detected in the spatially unresolved spectroscopic and broadband photometric observations of sun-like stars. In particular, observations of solar-type stars have now demonstrated that activity-related, irradiance variations are a universal property of a normal, solar-type star. Moreover, the level of activity is generally correlated with age. Young precursors to solar-like stars exhibit enhanced activity. This activity then declines with age in single (i.e., non-binary or multiple) stars.

In a study of nearby, solar-type stars, Lockwood *et al.* (1997) find that among stars with activity like the Sun average value, over 40% of the sample exhibited irradiance variations ranging from 0.3% to 1.2%, i.e., 3 to 12 times the amplitude of irradiance variations observed in the Sun (so far)! In fact, the irradiance variability of the Sun appears somewhat subdued for its level of activity (Radick *et al.* 1998). Whether the Sun is unusual in this regard is still a controversial point.

For solar-type members of the much younger, 0.6 Gyr old Hyades cluster, the *mean* level of cyclic irradiance variation is about 10 times the level of present-day solar variations (Radick *et al.* 1998). Thus, we infer that the ~0.5 Gyr -old Sun (end of the Hadean era) typically exhibited irradiance variability at a level that was an order of magnitude greater than what we see now. Even younger sun-like stars in the 100 Myr old Pleiades cluster are characterized by a mean level of magnetic activity that is ~6 times greater than the contemporary Sun. While irradiance monitoring of these stars over long time-scales has not yet been performed (an objective of this module), the predicted level of cyclic irradiance variability is about 2% or 20 times that of the present-day Sun.

2.4.2 Proposed Program

Effort (I): Visiting the epoch when the sun was young: Solar UV radiation plays a dominant role in the chemistry and dynamics of the earth's atmosphere. Moreover, the UV irradiance of the young Sun may have played a critical role in the origin of ozone and free oxygen in the prebiological paleoatmosphere of the earth (Canuto *et al.* 1983). Similarly, the nature of the habitable zones of young planetary systems, including the chemical evolution of young planetary atmospheres, will be impacted by the level and variability of the UV irradiance arising from magnetic field-related activity in the parent stars over both short and long (cycle-to-evolutionary) time scales.

We propose to establish an initial program to investigate the evolution of activity and the associated UV irradiance variations in solar-type stars spanning a wide range of ages. Of course, the UV emittance is not directly observable with ground-based telescopes. Therefore, our approach will rely on the observation of an accessible *surrogate* for UV irradiance in solar-type stars that are members of open clusters of known ages. These are the emission cores of the same H and K lines.

Knowledge of the variability of the Ca II H and K lines can provide an accurate estimate of the variations in the ultraviolet spectrum. Solar-type stars that are members of clusters, such as those shown in Figure 2.5, would be selected for long-term monitoring. The study of cluster members provides a stellar sample that is homogeneous in age and chemical composition. The mean level of normalized Ca II line emission in sun-like stars in clusters of known age is illustrated in Fig. 2.5 (adapted from Walter & Barry 1991).

While surveys of activity diagnostics in the visible, UV and X-ray have been performed for several young clusters (see Fig. 2.5), there is little information on the short-term excursions of activity (e.g., flares), which can occur, and no information on the nature of cycles (analogous to the solar cycle) in young (0.1 Gyr), solar-type stars. We would therefore utilize the MMT with the Hectechelle, or the WIYN telescope with the Hydra multiobject spectrograph, as appropriate, for Ca II H and K line observations of solar-type stars in selected clusters during one-night per month for at least 5 years, along with a parallel program of photometric monitoring with a GNAT (*Global Network of Astronomical Telescopes*) automated telescope. The results will yield quantitative insight on the nature of cycle-related activity—both UV and total irradiance variations---in solar-type stars at the young ages that presumably correspond to the early history in the evolution of planetary atmospheres. The most likely clusters for study are, in order of priority, the Pleiades (age ~ 0.1 Gyr), NGC 752 (1.7 Gyr), and the Hyades (age $\sim 0.7 - 1$ Gyr). Together with the M67 (age ~ 5 Gyr) program discussed in Proposed Effort (II), a complete

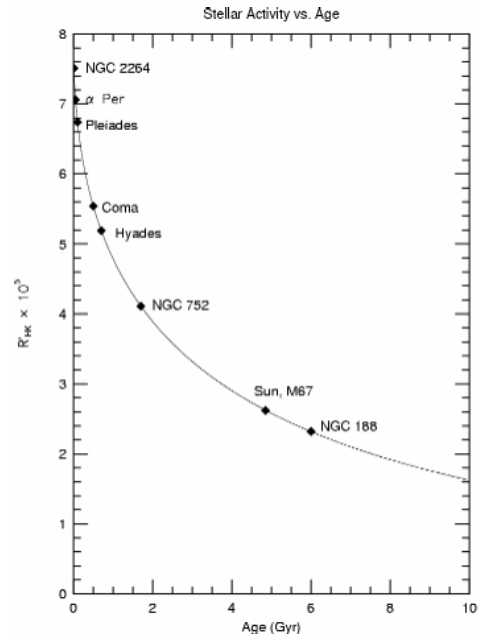


Figure 2.5. *The mean level of magnetic field-related activity of solar-type stars in open clusters of known age.* The index $R(HK)$ is the Ca II H&K line emission normalized by the stellar bolometric (total) flux and corrected for non-magnetic (photospheric) contributions to its total strength.

picture of the short-term and cycle-related variability of solar counterparts at ages ranging from 0.1 – 5 Gyr will be developed. Because of the development of photosynthesis during the Archean era (age 0.8 – 2.2Gyr) we will place emphasis on this era. We also propose a program aimed at understanding solar activity in the 0.01 to 0.1 Gyr range. Here, our focus will be on establishing the *range* in overall activity levels among solar-type stars during the epoch of planet-building and early planetary evolution. These results will provide critical context for the development of models of exoplanetary atmospheres during the early stages of planetary system evolution.

Effort (II): Placing the Mature Sun in Context: Our knowledge of the full range of solar variability that may occur is extremely limited. Given that individual solar cycles are different in form, amplitude and length, and because accurate solar data have been available only for the most recent cycles, there is no direct way of understanding *long-term* solar variability.

The observation of solar-type *stars* however, can be productively exploited to overcome the temporal confines of the solar database, thereby revealing the potential range and nature of *solar* variability over time scales that are simply not accessible to the modern solar database of only a few decades. We therefore propose to utilize the upgraded MMT with the Hectechelle multi-object spectrograph, along with an automated photometric telescope, to assemble a unique data set consisting of long-term observations of cycle-related, magnetic activity and associated irradiance variability in solar-type stars at various stages of evolution. The results will vastly increase our knowledge of the potential range of solar cycle-like variability on both short (~decades) and evolutionary time scales, from the very young Sun to the contemporary Sun. The resulting data can then be utilized as input for models of global climate change and for models of planetary atmospheres at various stages of evolution. In essence, we will delineate the nature and potential range of the joint variability of luminosity and activity experienced by “mature” planetary systems (including our own) bathed in the ambient and variable radiation fields of their parent suns.

As a first step toward understanding the nature and full range of variability of the contemporary Sun, we have completed a survey of the level of chromospheric Ca II H&K line core emission in the solar-type stars in the galactic cluster M67. This cluster is an especially appropriate object of observation since it is approximately the same age (about 5 Gyr) and has the same chemical abundances as the Sun. Our working hypothesis is that a single ‘snap-shot’ of a large sample of solar analogs reveals the potential range of *solar* chromospheric activity. In this way, we immediately obtain information on the potential *long-term* variability of the Sun that would not otherwise be possible (or practically feasible) with the modern solar Ca II data-base of only two decades. This is especially important given that the amplitude of long-term, solar and stellar variations in *brightness* are correlated with cycle variations in *chromospheric* emission (Hudson 1988; Radick 1991). In view of the fact that the Sun is the engine that drives climate on the Earth, any variation in the solar ‘constant’ must be taken into account in the investigation of the long-term behavior of the global climate.

In the M67 sample, there are 74 solar-type stars in the M67 sample with spectral types of G0 V - G9 V), corresponding to a range in mass of 1.10 - 0.95 solar masses (following Vandenberg & Bridges 1984). Among these stars are 21 “solar-twins” with intrinsic B-V colors between 0.63

and 0.67, which is the range of colors that has been quoted in the literature for the Sun as a star (VandenBerg & Bridges 1984, see their Table 2).

The results from the M67 survey of chromospheric activity in solar-type stars are encapsulated in the accompanying histogram (Fig. 2.6). The abscissa gives the H and K index, R , which is the flux in the Ca II H and K cores divided by the stellar bolometric flux. The R -values have been corrected for a non-chromospheric (photospheric) contribution (following Noyes *et al.* 1984). We display the distribution of this index for 74 solar-type stars in M67. The contemporary solar cycle is also shown, based on data obtained by W. C. Livingston (NSO/Kitt Peak) at the McMath-Pierce Solar Telescope facility of the National Solar Observatory on Kitt Peak from 1976 - 1994.

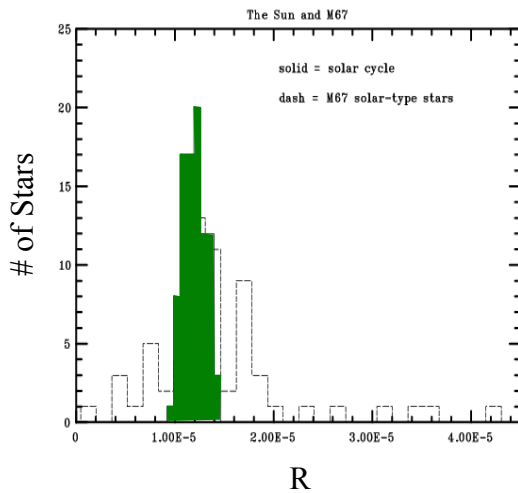


Figure 2.6. *The solar cycle and M67 solar-type stars with masses in the range of 1.10 – 0.95 solar masses.* About 18% of the solar analogs (colors $0.60 < (B-V) < 0.76$) exhibit especially quiescent levels of emission while about 32% display enhanced levels of activity compared to that at solar maximum. Of these, about 5% are an extreme state of activity.

The broader distributions in chromospheric Ca II strength for both the M67 solar-type stars, compared to that of the Sun during the contemporary solar cycle, suggest that the potential excursion in the amplitude of the solar cycle is greater than what we have seen so far. The stars with R -values noticeably less than solar minimum may be in a prolonged state of quiescence analogous to the Maunder-minimum episode of the Sun during A. D. 1645-1715 when visible manifestations of solar activity vanished. This period corresponds to a time of reduced average global temperatures on the earth known as the "Little Ice Age" (Foukal & Lean 1990).

Among the solar-type stars, about 18% are characterized by R values that are less than that estimated for the Maunder Minimum while approximately 32% exhibit R indices which are greater than that found at solar maximum. The Maunder-minimum value for R is derived from data given by Baliunas & Jastrow (1990) who, in turn, base their estimate on observations at the centers of solar supergranulation cells where the magnetic flux density is small.

In summary, we find that approximately 32% of the solar-type stars are in an enhanced state of magnetic activity while about 18% are at a significantly lower level--perhaps in a Maunder-minimum state. This could imply that the Sun spends nearly 50% of the time in a state of magnetic activity unlike what we have directly observed! Approximately 5% of the sample is in an "extreme state" of activity that could produce cyclic irradiance variations in the range of approximately 0.5% - 1% (i.e., 5-10 times the current solar levels), as inferred from the mean

relations of cyclic photometric variation versus mean chromospheric activity given by Radick *et al.* (1998). About 24% of the M67 solar counterparts are in an "enhanced activity" state with an estimated amplitude of irradiance variability of $\sim 0.2\%$, or two times that of the Sun.

Given the positive correlation between magnetic activity and brightness changes, our results suggest that the total solar irradiance could change by more than the 0.1% currently observed! This could, in turn, have significant implications for climate change over century-long time scales. In fact, a change of only 0.22-0.55% has been estimated to lead to a change of 0.4-0.5 degrees C in global mean temperature (Wigley et al. 1990).

These intriguing results pose crucial questions. In particular, is the stellar distribution in the figures really the result of the modulation of activity by cycles analogous to the solar cycle, or are the *relative amplitudes* of the cycles actually similar with the differences due only to differences in the *mean level* of activity among solar-type stars? Even more fundamentally, is the distribution of chromospheric H&K emission strength arising from solar-like cycles at all? The only way to address these critical issues is to obtain regular observations of the M67 "Suns" over a period of several years.

We propose to implement a long-term program of H&K observations during each bright run during the M67 observing season (about Dec. - Apr.). Specifically, we would utilize the MMT with the Hectechelle one-night per month for at least 5 years and preferably 10 years (about the length of the sunspot cycle).

We will establish a parallel program of photometric monitoring using an automated telescope in order to obtain data on the associated luminosity variability of the program stars. The telescope is a facility of the Global Network of Automated Telescopes, Inc., in Tucson, Arizona.

The results will enable us to build a statistical picture of all the modes and amplitudes of the cycle variability of solar-type stars and, by inference, of the Sun itself. Of equal importance, they will provide valuable input for the construction of global climate change models.

Module 3: Characterization of Planetary Systems

Team: R. Angel (Lead), A. Burrows, L. Close, P. Hinz (Deputy), J. Lunine, M. Meyer, and N. Woolf

3.1 Introduction

Our solar system may be only one many planetary systems in the neighborhood of our sun capable of sustaining life. We propose to further our knowledge of where planetary systems exist in the solar neighborhood, including the nearest star formation regions. We want to discover the range of planetary systems, the frequency of types, and study how likely they are to be abodes for life outside our solar system. The work is directed towards Goal 1 of the Astrobiology road map, and in particular towards goal 1.1, though it also impinges on goal 1.2.

We also plan to study the spectrum of the whole earth observed from earthshine on the moon. We want to discover the spectral characteristics of those regions not well studied, and to observe the time variation of features to understand the problems and issues in interpreting the spectrum of earth as a whole. This work is directed towards goals 1.2 and 7 of the Astrobiology road map.

3.2 Planet Searches

Jovian planets are the alpha and omega of planetary system evolution. They control whether terrestrial planets form, the abundance of volatiles on these planets, and the frequency of violent impacts on them after formation. We want to image giant planets directly, to discover planetary systems of kinds that cannot currently be found.

We are looking for gas giant planets, and particularly for a change in the frequency of these planets beyond the ice line. We take this to be at a distance $5(L/L_{\text{sun}})^{0.5}$ AU from a star. We expect such a change if "radial velocity planets" are a minor group compared with "solar system-like planets" with similar orbital parameters. Our proposed techniques are:

1. Directly image massive planets orbiting nearby 0.1-10 Gyr old "Sunlike" stars. This challenging task will be accomplished utilizing two complementary and novel imaging techniques (3 color simultaneous differential CH₄ imaging and nulling interferometry) with Arizona's Monolithic Mirror Telescope (MMT) and Large Binocular Telescope (LBT);
2. Probe the physical properties of these planets and systems through photometry and spectroscopy. Our goal will be to use the photometric data to infer the luminosities of planets. Combined with the known age of the system, this leads to mass estimates. By comparing synthetic spectra of giant planet atmospheres with observations of the planets we can constrain the planet mass. These data, combined with the orbital information gathered and dynamical simulations outlined in Module 2, will enable us to assess the potential of systems to have terrestrial planets with volatiles.
3. Through this we will help lay the technical and theoretical foundations for successful surveys for life bearing worlds to be undertaken with the Terrestrial Planet Finder and its precursor missions.

We also want to learn about the potential for planets with a water-atmosphere boundary. In Jovian planets we expect to find parts of the atmosphere where water is present in droplet form. In some lower mass planets we may find a water layer sitting on a rocky core. This potential for "super-earths" needs exploration, and we will start moving towards it by modelling planets down to 0.1 Jupiter masses.

In addition to searching for other planets by learning about the frequency of potentially habitable nearby planetary systems, we want to make more studies of the one planet we know to be both habitable and inhabited - Earth. We want to learn more about the problems of observing the changing spectrum of the earth using earthshine and the issues in interpreting a crude spectrum such as we would expect to get from Terrestrial Planet Finder.

Our efforts here are part of a long-term strategy to insure success (or place meaningful limits) in the search for life beyond the solar system. We were first in proposing schemes for the detection of terrestrial planets in the mid-IR. We were first to examine the requirements for an adaptive optics system to find planets around other stars. We proposed the re-direction of the search for Jovian planets towards young planets in our NRA study - "Self-Luminous Planet Finder". We will continue to develop novel ideas to solve daunting problems associated with the search for the origins of stars, planets, and life. Support through this program will insure that we focus our efforts in areas that are most likely to be interesting to astrobiology.

3.3 Planet Searches at the University of Arizona

The University of Arizona is well suited to carry out astrobiological inquiries into massive planets and their influence on extra-solar planetary systems. Arizona arguably has one of the strongest interdisciplinary synergies between telescopes, instrumentalists, observers, planet modelers, planetary system modelers and TPF experts.

The synergy from these interdisciplinary groups will enable an astrobiology program at the University of Arizona to make breakthroughs into studies focused on the nature, frequency, formation, and evolution of planetary systems where massive gas giants point to the presence of habitable terrestrial planets.

3.4 Science goals

In this module we propose to explore directly the frequency of giant planets around other stars near the Sun, and relate this to the conditions in the so-called "habitable zone," where life might exist if solid (terrestrial-type) planets are present. We plan to combine the observations of Hinz, Angel, Close, and Meyer and TPF studies of Woolf, Lunine, Angel, and Hinz with the atmospheric and dynamical modeling expertise of Burrows and Lunine to address the following list of questions:

1. What is the lowest mass planets that we can discover through direct imaging, both for star formation regions less than 10^7 years old, and for nearby stars where the answers are better known. Based on these observations we can start to answer:

2. What is the frequency of giant planet formation and, in particular, how often do Jovian planets form in a planetary system (*i.e.*, compared to higher mass sub-stellar objects)? Do the spectral properties of these objects fit the current models? What are their masses? Do follow up observations suggest circular or highly eccentric orbits? Given this newly characterized distribution of "wide" (~3-50 AU) giant-planet objects, combined with the known "tight" (0.05~3 AU) radial velocity/transit planets, we then ask:
3. What are the habitable zones for the new systems compared to the radial velocity systems?
4. What are the spectral signatures of terrestrial planets orbiting at various thermal environments around stars? What are the characteristics of life and habitability signatures on "super earths"? To what extent will biospheres develop obvious biosignatures? To what extent will there even be habitability signatures? What spectral evidence do we search for to identify acquired volatiles? What do young terrestrial planets in their Hadean era – up to 5×10^8 years old – versus older terrestrial planets in Archean versus Proterozoic and later eras – 10^9 to 10^{10} years – look like? How might habitability be mimicked by terrestrial planets undergoing unstable, dynamical episodes of atmospheric evolution or loss or ice-ball episodes? Finally, to broaden the search for habitable places in the cosmos, we ask:
5. Given the properties of detected giant planets (spectral type, atmospheric composition, temperature, mass, radius, semi-major axis, stellar type and age of parent), what is the full range of habitability possibilities around these objects? That is, might the giant planets have habitable moons, or even be habitable themselves? Is there a biochemical distinction between habitable moons with an ice layer over their water and ones with a water-atmosphere boundary? Ultimately, regardless of whether habitable moons exist around giant planets, we wish to characterize their spectral properties both to understand the range in giant planet atmospheric compositions, and as a pathfinder to doing the same for terrestrial planets. Hence:
6. What key spectral features might be detected in next-generation images of extra-solar planets and what are the key properties we seek in such giant planet spectra?

3.5 Observational Detection of Other Planetary Systems

In this section we outline the facilities and observational programs planned to further our knowledge of the makeup and habitability of other planetary systems. We describe two specialized techniques planned for detecting companions within the region of expected planet formation (1-40 AU): simultaneous differential imaging (section 3.5.2) and differential imaging (section 3.5.3). Simultaneous differential (Sim. Diff.) spectral imaging at $1.6 \mu\text{m}$ is expected to be most useful for finding and characterizing young planetary companions. Nulling interferometry will be important at $5 \mu\text{m}$ to detect older (and thus cooler) planets.

3.5.1 Facilities for Extrasolar Planetary Searches

Arizona has pioneered both the development of large-aperture telescopes and an implementation of adaptive optics (AO) most suited to planet searches. Because of the difficulty in detecting faint planetary companions next to bright stars in observations limited by the atmospheric blurring known as "seeing", techniques to control the wavefront distortions caused by the earth's atmosphere known as "adaptive optics" have been developed. Corrections to the wavefront are achieved by monitoring the distortions many times per second and using a deformable mirror whose shape is altered on similar timescales. By integrating the correcting element of the AO system into the telescope itself (as its secondary mirror) both the sensitivity and the image of the sharpness can be maximized.

The 6.5 m MMT (in which Arizona is a 50% partner) is the first realization of a large aperture telescope coupled with a deformable secondary. Figure 3.1 shows an image demonstrating the successful use of the MMT AO system to create ultra-sharp images by correcting the atmospheric turbulence. The system allowed images to be made with 40% of the object's flux in a diffraction-limited core of size $0.050''$ at $1.6 \mu\text{m}$. At longer wavelengths the MMT achieves even higher amounts of light in the core $\sim 98\%$ with a FWHM = $0.32''$ at $10 \mu\text{m}$. Concentrating the blur of these point sources of light is central to optimum detectability. These angular scales correspond to separations of 0.5 AU and 3.2 AU respectively between a host star and any potential planetary companions.

At longer wavelengths ($>2.5 \mu\text{m}$) the MMT AO system is uniquely sensitive, due to the lower background light it emits at infrared wavelengths compared to conventional AO systems. This is because it uses a deformable secondary mirror for wavefront correction (Brusa *et al.*, 1999) which has the advantage of eliminating ~ 8 warm, dusty, optical surfaces from the AO system design (Lloyd-Hart, 2000). The elimination of these extra optical surfaces (that are required of all conventional large telescope AO systems – *e.g.*, Keck, VLT, *etc.*) allows the MMT AO to have much lower scattered light, and lower thermal emissivity, while increasing the system throughput. Conservative estimates of this suggest that 6.5 m MMT AO system in conventional imaging mode will be ~ 1.0 times as efficient as the Keck (10 m) AO system at H ($1.6 \mu\text{m}$) and 2.28 times as efficient at N ($10.5 \mu\text{m}$) despite having a smaller primary mirror (for more on the MMT AO system see Lloyd-Hart, 2000; Wildi *et al.*, 2003). Arizona is also a partner in the Magellan 6.5 m southern telescopes, and we expect to create a similar adaptive

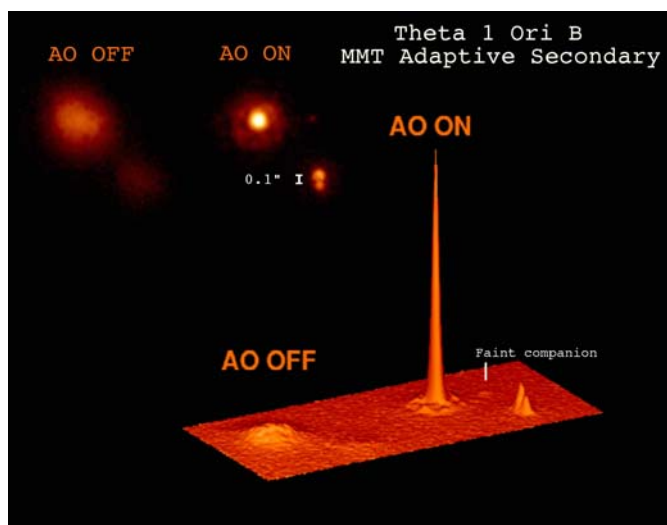


Fig. 3.1. Demonstration of the MMT adaptive optics system to create diffraction-limited images at $1.6 \mu\text{m}$. We see that with the AO correction "OFF" faint companions are impossible to detect (upper left), whereas with AO "ON" all four stars (in the theta 1 Ori B group) become clear. Adaptive optics correction is the first step in being able to directly image extra-solar planets.

secondary system for one of these telescopes.

Arizona is also a 25% partner in the Large Binocular Telescope, a 2×8.4 m telescope with uniquely sensitive planetary detection capabilities. NASA has already recognized this in its funding of the LBT Interferometer (LBTI) as part of the Navigator Program. The development of the LBTI is being funded to further technological development for the Terrestrial Planet Finder Program, through the demonstration of nulling interferometry. We want to use the already-funded facilities of this NASA program to make surveys for extrasolar zodiacal dust (module 2) and giant planets focused on the astrobiological issues. The secondary mirrors of the LBT will, like the MMT, be deformable for AO wavefront correction. The increased collecting area as well as greater angular resolution of the LBT will allow us to study planetary systems found with the MMT in greater detail as well as extend our searches to fainter (and thus less-massive planets).

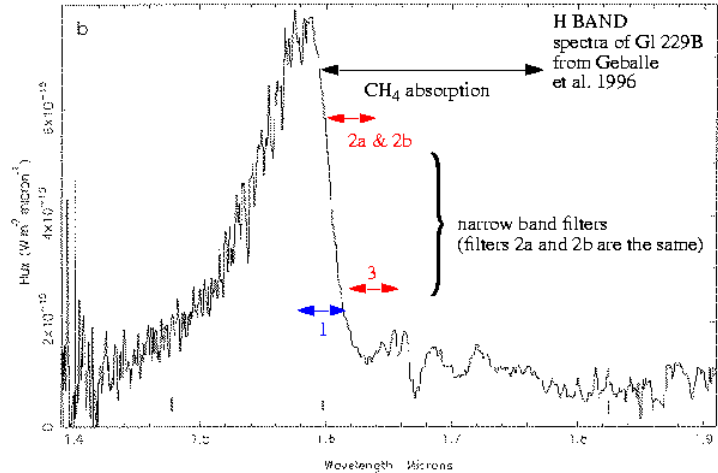


Figure 3.2. All planets between 1300-400 K will have strong CH_4 absorption. We have built an adaptive optics instrument (a 3 color Sim. Diff. Imager in the ARIES camera) with filters 1, 2a, 2b, & 3 on either side of the CH_4 absorption. Subtracting images made in these filters will remove the star but leave the planet's image to be detected.

3.5.2 Three Color Simultaneous Differential Imaging

We have developed a new technique that is a variant of the simultaneous differential imaging technique of Rosenthal *et al.* (1996), Racine *et al.* (1999), and Marois *et al.* (2000). The technique is designed to detect a companion close to its parent star by taking advantage of the difference in brightness of the planet at two closely spaced wavelengths. This allows one to achieve a gain in limiting sensitivity over normal imaging by ~ 20000 times. The 3 color technique is photon-noise limited for separations of $>0.2''$. For the first time massive planets in the range 5-13 M_J , at distances 5-30 AU from young (0.1-1 Gyr) Sun-like stars, within 50 pc of our solar system, can be directly detected and imaged.

3.5.2.1 How three color simultaneous differential imaging works

The simultaneous differential imaging works by means of creating 4 images of the same star in 3 different wavelengths simultaneously. As Fig. 3.2 shows we plan to have 3 different filters that will sample either side of the CH_4 absorption feature at $1.61 \mu\text{m}$. A subtraction of these filters will remove the starlight but reveal the massive planet. It is important to note that all massive planets from 1-13 M_J and from 0.1-5 Gyr have strong CH_4 absorption at $1.62 \mu\text{m}$ (Burrows *et al.*, 1997). Therefore, differential CH_4 imaging is a powerful technique to detect massive planets over a wide range of ages and masses.

Early experiments with CH₄ differential imaging were made at the CFHT 3.6 m telescope with the MONICA 256 x 256 IR camera and the PUEO AO system (Racine *et al.*, 1999). These experiments proved that gains of ~50 in the sensitivity were obtained when using 2 colors and subtracting images at 1.5 μm from images at 1.7 μm. This is, however, nowhere near the improvement needed to reach the photon-noise limit of a deep exposure ~400x more rejection of the primary's starlight is required. To get this extra rejection of the primary's contaminating "wings" requires a more complex subtraction process less prone to systematic errors between the "out" and "in" CH₄ images. To achieve a higher rejection we will use 3 colors and 4 images (instead of the previously used 2 colors and 2 images) and will obtain a final image by differencing the differences between the pairs of images. This in effect improves upon previous techniques by removing second-order systematics resulting from the wavelength dependence of the speckle pattern.

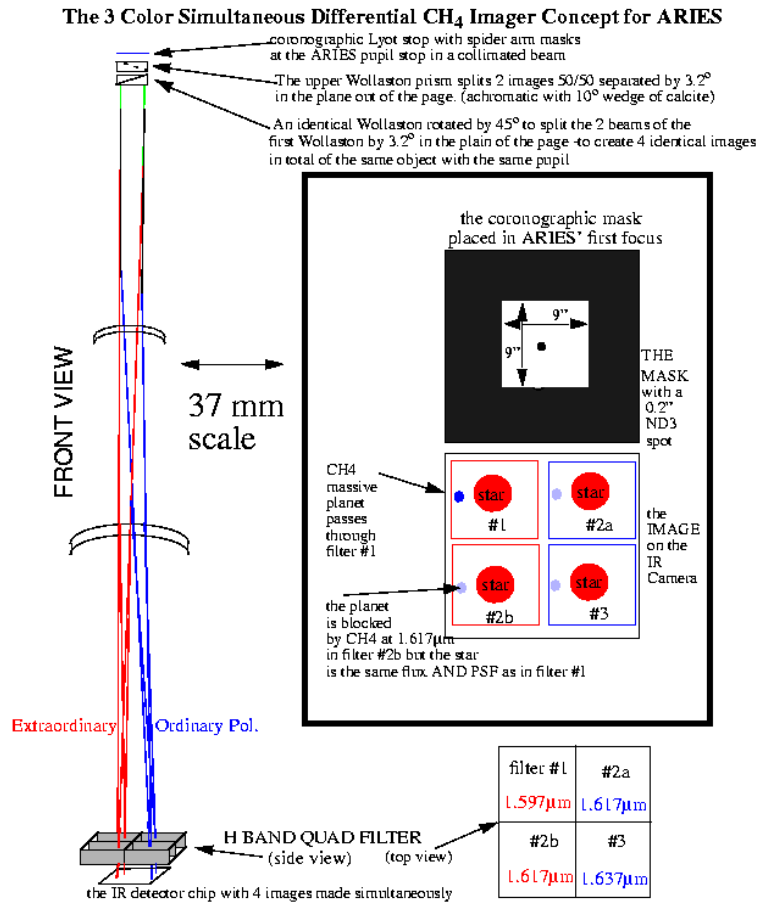


Figure 3.3. A schematic diagram of the instrument built for the MMT adaptive optics telescope. This instrument (hosted inside the ARIES infrared camera) is operating in the lab. It allows for the direct detection of gas giants for the first time.

3.5.2.2 Status of 3 color simultaneous differential imaging

The differential imager instrument has been tested cold (77 K) in the ARIES science camera dewar for use with the MMT AO (see Figure 3.3; Freed *et al.* 2003). Our first telescope observations could occur in May 2003. However, our lab data already show that our instrument is performing as expected (at the photon-noise limit). Based on laboratory experiments we believe we can detect planets 10,000 times fainter than the primary star at just 0.4" from the star (10 AU if the star is at 25 pc from the Sun) in only 5 seconds of integration at the MMT. In 2 hours of integration at the photon limit we should detect planets 100,000 times fainter than the primary at the MMT at the 10σ confidence level. This is >1000 times more sensitive than what has been possible before from any space or ground based telescope at 0.4" separations (Close 2000). Based on these measured lab sensitivities and the planetary models of Burrows *et al.* (1997) we show in Figure 3.4 our predicted sensitivities to extra-solar planets for several different primary star types and masses.

3.5.1.3 The proposed 3 color Sim. Diff. surveys

We propose to capitalize on this sensitivity and efficiency to carry out the first large, deep, 3 color differential CH₄ (methane) AO survey of nearby stars. The survey will characterize companions about both nearby mature stars and younger stars.

Survey #1: MATURE STARS: A Complete survey of all 100 known (from NSTARS- Henry *et al.*, 1998.5) northern hemisphere stars between 0.5 and 1.5 M_{Solar} within 10 pc. In two hours of integration we will be sensitive down to planets of magnitude $H = 26$ (corresponding to 5 M_J surrounding 5 Gyr old stars at 5 pc from the Sun). We will obtain deep two hour images of the nearest stars with DEC > -25° to extend massive planet searches down to planets of H~26, ~100 times deeper than has been attempted before. We will detect planet masses of 7 M_J at 5 AU around a 5 Gyr star at 5pc. In general, this photon-noise limited survey will be complete for older ~1.0-10 Gyr old (mature), massive planets of ~5-80 M_J with semi major axis of ~5-90 AU.

Survey #2: YOUNG STARS: Image all 60 young (<1.0 Gyr; age based on CaII H and K emission survey of Soderblom *et al.* (1994)) stars that are nearby (D < 25 pc). We should be sensitive to 3 M_J objects at 5 AU from a 300 Myr old G2V star at 5 pc in two hours. Although there may not be as many of these young nearby stars, they will certainly be good targets for direct detection of lower mass planets. The radial velocity planet confirmed around ε Eri (after 15 years of radial velocity observation is observed to have mass ~4 M_J (assuming a nearly face-on orbit), current separation ~0.5", D = 3.3 pc, age ~ 700 Myr) would be relatively "easy" to image in two hours and is a good example of a potentially accessible planet for detailed study.

3.5.3 Nulling Interferometry Detection of Giant Planets

Nulling interferometry is a technique which is central to NASA's plans to look for life around nearby stars, through the Terrestrial Planet Finder mission. It allows the detection

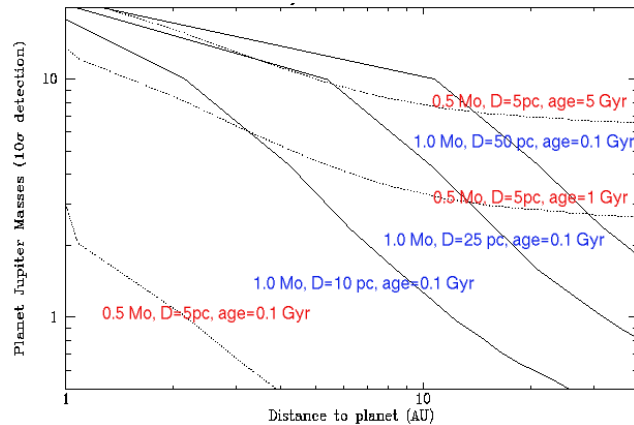


Figure 3.4. The sensitivity of the 3 color Sim. Diff. Imager to planets (at a very high 10 σ level of confidence) orbiting different primary star masses (0.5 or 1.0 solar masses (Mo)), ages (0.1-5 Gyr), and distances (5-50 pc). This assumes 2 hours of integration per star at the MMT 6.5m telescope.

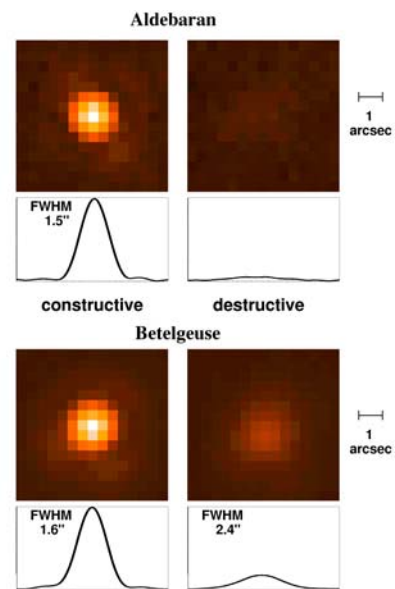


Figure 3.5 The first demonstration of nulling interferometry with the Multiple Mirror Telescope. The star Aldebaran is effectively suppressed in the right top image by destructively interfering light from two telescopes. In contrast, when the star Betelgeuse is suppressed an extended image remains, which is a direct image of the dust nebula surrounding the star. The nebula is not suppressed since it is much larger than the stellar disk of Betelgeuse.

of faint circumstellar material or object in the presence of the much brighter stellar emission. We first demonstrated nulling interferometry to be capable of directly imaging faint circumstellar environments (Hinz *et al.* 1998) using two of the six mirrors of the old Multiple Mirror Telescope (now refurbished as a single 6.5 m telescope). The two pupils were overlapped so that the starlight combined out of phase, canceling out in the image. Light from a source elsewhere in the image does not combine out of phase and can thus be seen even if it is intrinsically much fainter than the nulled out star. The results of this first test are shown in Figure 3.5.

With the deformable secondary, suppression factors of 10,000 will be possible while still maintaining optimum sensitivity in the thermal infrared (Hinz *et al.* 1999). This combination will allow detection of very faint circumstellar objects and structure.

3.5.2.1 Status of nulling interferometry with the MMT and LBT

We have completed a nulling interferometer for use with the 6.5 m MMT and Magellan. The instrument was first tested in January 2003. The instrument is designed for use both at 10 μm wavelength (where we expect to use it for detection of zodiacal dust, as described in module 2) and at 5 μm for detection of giant planets.

The Large Binocular Telescope, currently near completion on Mt. Graham in Arizona, will be a uniquely powerful nulling interferometer. The 8.4 m primaries, center-to-center separated by 14.4 m, on a common telescope mount with deformable secondaries all contribute to form an interferometer which is sensitive in the infrared and capable of deep stellar suppression. Full interferometric operation of the LBT is planned by October 2005. We are currently building the nulling interferometer for the LBT (NIL) which has benefited from our experience with nulling on the MMT. Nulling is a technique most easily performed in the thermal infrared (4-13 μm). Here the noise source is different than in the near infrared (1-2 μm). Through nulling, scattered starlight and speckles associated with it are reduced to well below the noise level associated with the background light contributed by the sky and the warm telescope mirrors. For this situation the MMT AO system is advantageous, not only for the better PSF it produces, but because it does not introduce any extra warm mirror surfaces which glow in the infrared, adding extra background light. This allows us to have a very sensitive system. Other interferometers will have many warm reflections prior to combination of the light. Extra mirrors are needed both for conventional AO systems and for movable delay lines required in interferometers which are not mounted on a common structure as is the LBT. We estimate the sensitivity of the MMT nulling interferometer to be able to detect a 200 microJansky source at 5 μm and a 900 microJansky source at 10 μm for a 1000 second integration (Hinz *et al.* 1999). The LBT will improve on this, detecting 30 microJansky sources at 5 μm and 150 microJansky sources at 10 μm . We relate these sensitivity numbers to detectable objects below.

3.5.3.2 Nulling survey for detecting giant planets

Surveys undertaken with nulling both at the MMT and the LBT will have two separate objectives related to extrasolar planetary systems: detecting zodiacal dust disks at 10 μm , where they are relatively bright (which is addressed in module 2), and detecting extrasolar giant planets. Direct detection of a companion is more feasible in the thermal infrared than the visible or near infrared, since the planet's thermal emission in the infrared is brighter, in comparison to the

stellar emission, than the amount it reflects in the visible or near-infrared. However, by looking for a planet in the infrared where it is emitting its own radiation rather than the reflected light from its star, the detectability of a giant planet is sharply dependent on how old it is, and thus how much it has had a chance to cool.

We have used the models by Burrows et al. (1997) to determine planet detectability. Figure 3.6 shows an interpolation of the Burrows *et al.* predictions for a 5 Jupiter mass object at 10 pc from an age of 0.1-1 Gyr in the N, M, and L' bands along with the plotted MMT sensitivity limits. From these it is possible to derive mass limits for detection with each instrument. The photometric sensitivity for the MMT allows us to detect 4 Jupiter mass planets 0.5 Gyr old, 6 Jupiter mass planets 1 Gyr old, and 15 Jupiter mass planets 5 Gyr old for stars 10 pc away. For the LBT the numbers are 1, 2, and 5 Jupiter mass objects for the respective ages. These numbers are expected to be only mildly dependent on the planet-star separation. The closest separation nulling can sense is determined by the separation of the apertures, and is 0.10" for the MMT and 0.027" for the LBT in the L', corresponding to 1 and 0.3 AU, respectively, at 10 pc. The outer limits are set by detector area and are expected to be 130 and 35 AU respectively.

In support of this proposal we will conduct nulling surveys at the MMT complementary to the differential imaging survey outlined above: first observing a volume-limited sample of 100 nearby stars and then extending our approach to the nearest 60 young solar-type stars. Follow-up observations of companions detected with the MMT will be carried out with the LBT, which will have the ability to obtain low-resolution spectra of any object detectable with the MMT.

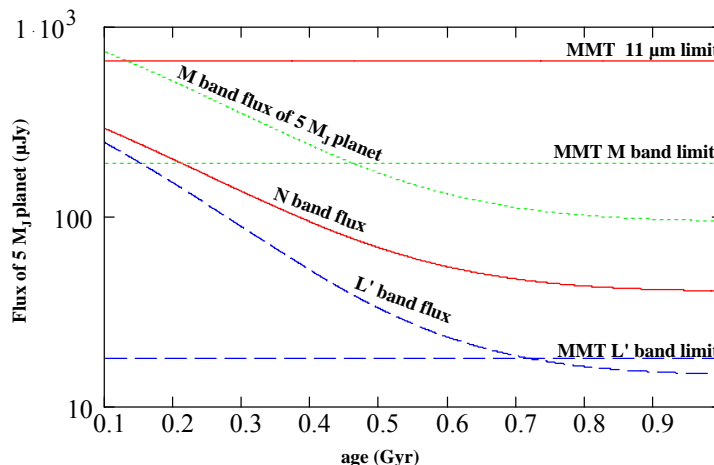


Figure 3.6. Detectability of planets in the N (11 μm), M (4.8 μm), and L' (3.8 μm) bands at the 6.5 m MMT. The fluxes, from Burrows et al. (1997), are for a 5 Jupiter mass at 10 pc. The planet is most readily detectable in the L' band

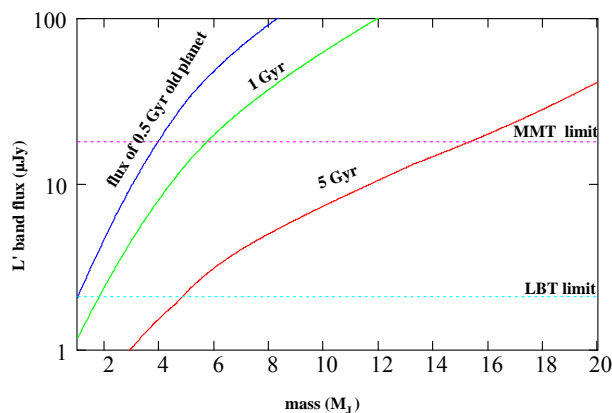


Figure 3.7. Minimum planet mass detectable at L' for the MMT and LBT. Fluxes are for planetary systems at 10 pc from Burrows et al. (1997).

Direct detection of planets is not a mature field. Although much effort has gone into developing a variety of techniques, no one approach has emerged as uniquely successful in detecting faint substellar companions. We have outlined a multi-faceted approach for the direct detection of extra-solar giant planets, each searching a specific range of parameter space in complementary ways. In this way, we hope to provide observational constraints that will help answer aspects of the fundamental questions: where, when, and how frequently giant planets form around solar-type stars.

3.6 Giant Planet Modeling

In the last seven years, more than 100 extrasolar giant planets (EGPs) have been discovered by precision radial-velocity measurements of the telltale wobble of their central stars, and their discovery constitutes a major turning point in both planetary science and astronomy. The unanticipated variety of these extrasolar planetary systems (most completely unlike our own) has upended conventional wisdom concerning the formation of planetary systems and is drawing an increasing fraction of the world's astronomers into the technological, theoretical, and observational programs designed to study and understand them in more detail.

Although the radial-velocity programs have launched the modern study of EGPs, it is only by making *direct* measurements of the planet's spectrum that its physical characteristics can be fully discovered. Hence, the next stage after the initial ground-breaking Doppler campaigns in the study of EGPs will be their direct imaging and spectroscopic measurement. The theoretical modeling of EGP atmospheres is important for at least two major reasons. First, since the emergent spectra of EGPs are determined by the chemistry and physics of their outer atmospheres, when direct detection of EGPs is achieved and spectra are obtained, theoretical models will be essential in the interpretation of the data and in the extraction of essential physical information such as radius, gravity, temperature, and composition. Then in turn the verified characteristics can be used to determine masses of planets that do not have a radial velocity signature. This is the essential key to exploring the nature of planetary systems.

Second---and this is perhaps the more pressing of the two---theoretical spectral models are important in guiding current and upcoming direct EGP searches. Observers need to know which regions of the spectrum provide the greatest chance for detection, while avoiding those regions in which attempts are likely to be futile. The two observing techniques outlined above illustrate this; both the methane absorption and 5 μm feature are well modeled by our current spectra, and are providing input for estimated sensitivity in both cases.

We (Sudarsky, Burrows, and Hubeny 2003) have already conducted an extensive exploration of spectral and atmospheric models of irradiated extrasolar giant planets. Our central purpose has been to provide a map to observers, as well as a comprehensive view of the theoretical possibilities. We have investigated the dependence of the phase-averaged emergent spectra on orbital distance, stellar type, the presence or absence of clouds, cloud particle sizes, surface gravity, and the inner flux boundary condition. Included are calculations for irradiated brown dwarfs, specific known EGP systems, and a generic sequence around a G0V star. The hot planets give information that helps the understanding and modeling of those planets which will be in potentially life bearing planetary systems.

There are many overall, as well as specific, conclusions resulting from the current state of modeling. Some of the more salient points are the following:

1. The planet-to-star flux ratio is a very sensitive function of wavelength and orbital distance.
2. EGP band fluxes are not strictly monotonic functions of orbital distance, nor are the Bond and geometric albedos.
3. EGPs fall naturally into classes due to qualitative similarities in the compositions and spectra of objects within several broad atmospheric temperature ranges.
4. The mid-infrared region of the spectrum from 10 to 30 μm has a favorable planet-to-star flux ratio, even for distant EGPs.
5. Due to Rayleigh and/or grain scattering, the optical spectrum of an irradiated brown dwarf can be very much brighter than that of a brown dwarf in isolation, even when its near- and mid-infrared spectra remain relatively unaffected.
6. Fluxes in the *Z*, *J*, *H*, and *K* bands of an EGP in a long-period orbit can be enhanced above baseline levels (normally determined by stellar irradiation and scattering alone), if the planet is either young or massive.
7. There is a *relatively* bright feature within the 3.8 to 5 μm wavelength region for all irradiated EGPs, and in particular for the more distant EGPs (such as 55 Cnc d, ϵ Eridani, 47 UMa c, Gliese 777A, and υ And d).
8. As a result of the progressive decrease in atmospheric CO abundance, the center of the 3.8 to 5.0 μm feature shifts systematically from shorter to longer wavelengths with increasing orbital distance (or decreasing stellar luminosity).
9. Rayleigh and grain scattering elevate the optical and near-IR fluxes, but grain absorption depresses the mid-infrared fluxes (in particular in the "5- μm " band).
10. Increasing surface gravity slightly decreases the flux shortward of ~ 2.2 μm , but also slightly increases it longward of ~ 2.2 μm . The larger the gravity the smaller the peak-to-trough variations throughout the spectrum.
11. The Na-D and K I resonance doublets are prominent features of the hottest, close-in EGPs (such as 51 Peg b, τ Boo b, HD209458b), but quickly wane in importance with increasing orbital distance.

However, much remains to be done. At low effective temperatures (< 400 K), water vapor condenses into water clouds in both irradiated EGPs and brown dwarfs. The formation of clouds of this sort is one of the first markers of planet-like behavior as seen in the Solar System are familiar and ties the physics of our nine planets and their moons with that of extrasolar giant

planets and brown dwarfs. Objects less massive than $\sim 20 M_J$ will in a Hubble time or less achieve sufficiently low effective temperatures (T_{eff}) for water clouds to be manifest. Such objects could exist either as free-floaters in the ISM and be detectable by SIRTf, JWST, and TPF or could be bound in orbits around nearby stars. The latter "planets" are subject to irradiation and will have distinctly different spectra and colors.

In this proposal, we will extend the theory already developed for the known EGPs and brown dwarfs to lower T_{eff} , gravities, and masses to include the onset of water cloud and ammonia cloud ($T_{\text{eff}} < 200 \text{ K}$) formation. This will include objects as small as $0.1 M_J$. The technology to do this is already in hand. It will be used to make predictions in support of our local observational efforts, as well as those of the international community via the variety of telescopes now being designed for the direct characterization of planets outside our solar system. The study of the lower mass objects will start the exploration of the character of "super earths", Uranus-Neptune mass objects at greater irradiance.

3.7 Terrestrial Planet Finder Preparation and the Earth spectral signature

Ultimately spaceborne platforms will be built that are capable of detecting, and collecting spectra of, terrestrial planets. We currently do not even have adequate information about the spectrum of the earth, or its time variability. We have already made observations of lunar earthshine (Woolf *et al.* 2002) as shown in Figure 3.8. We discovered that our modeling had missed a most

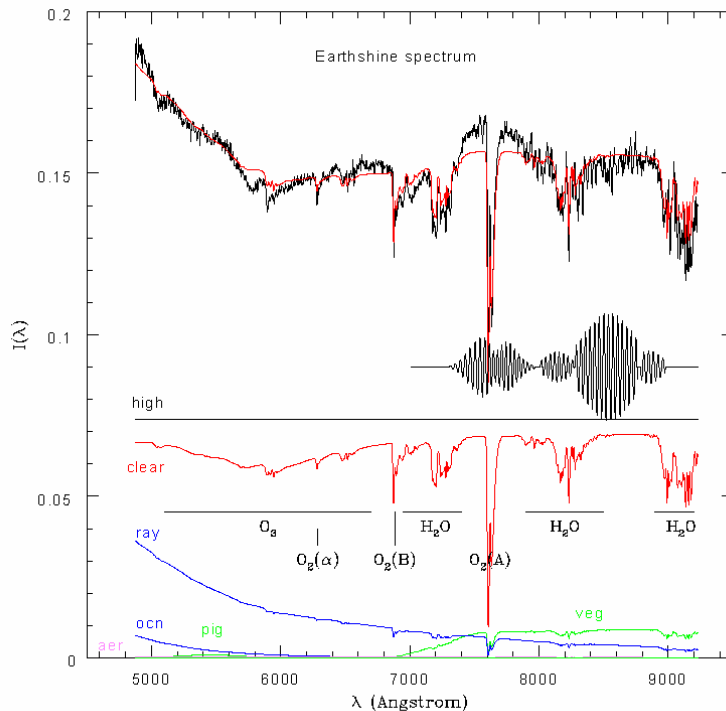


Figure 3.8. The earth's integrated reflectivity versus wavelength determined from lunar earthshine. The blue "ray" curve is the extracted Rayleigh scattering component. The green "veg" curve is the extracted vegetation signature, though there are indications in the 7500-8000A region that this component is stronger, and with a different signature than we have used in the analysis.

significant feature - the Rayleigh scattering of the atmosphere. This is an essential tool to interpret the molecular spectral features in the atmosphere. Without it we cannot determine whether features are strong because of the abundance of the molecules, or because of collisional broadening. Unsaturated features, that have for example allowed us to infer the presence of water and CO₂ on Mars, are too weak to be visible in spectra we expect from external planets.

The Rayleigh scattering would be straightforward to interpret as atmospheric pressure in a clear atmosphere, but in the presence of cloud the results are more complicated. We would like to model the effect of clouds, and make observations to see how the Rayleigh scattering changes with time, using weather maps to tell whether we have the story correct.

The vegetation red edge only measures land plants because seawater has a very strong absorption in this spectral region. The signature is not expected to be unique, as e.g. bacteriochlorophyll would produce a red edge beyond 1 micron. However the inefficiency of biological processes, and the susceptibility of land plants to overheating, makes it seem plausible that oxygenic photosynthesis land organisms on another planet will also have a red edge in this general wavelength region. We would like to study this issue further, by collaborating with oceanographers at other NAI nodes to compare the spectral characteristics of green algae, red algae and brown algae. We want to know whether their absorption at ~ 8000Å differs and makes the green algae less susceptible to desiccation and so selected the green algae to be the ancestors of land plants.

The spectral region from 1-2.5 μm is not yet known in a whole earth spectrum, and we propose to observe it on the VATT telescope on Mt. Graham, where we now have an appropriate spectrograph. (An earlier request for time on IRTF for this work was denied). We think that there may be some indicators of the kinds of bare rock and sand in Earth's desert regions in this part of the spectrum.

We are also interested in finding about the variability of the Earth spectrum, and the visible spectrum is highly time variable. We will find if it impinges on analysis of results if the TPF mission is designed for the visible spectral region. Fortunately, we already have a good whole-earth spectrum of the mid IR region from TES spacecraft, and this will have less variability.

3.8 Summary of Module 3

Products of the observational effort will initially be discoveries of >Jupiter mass objects around nearby Sun-like stars ($0.5 < \text{mass} < 1.5M_{\text{Solar}}$) and younger. Our first survey of 100 nearby (1-10 pc), mature (1-5 Gyr old) stars will be sensitive to massive planets of 5 M_J at $r > 5$ AU at 5 pc. Our second survey of 60 younger (<1 Gyr - CaI selected objects) will be sensitive to massive planets of 3M_J at $r > 5$ AU at 5 pc. Each massive planet detected will have photometric and spectroscopic follow-up observations to characterize its mass, temperature, luminosity, albedo, composition, and surface gravity. From our final "catalogue" of massive planets we will distill the frequency of massive companions as well as the semi-major axis distributions and mass distribution of these objects (taking into account the selection bias of our well designed samples). Our goal is not just to observe single planets but to determine the characteristics of planetary systems.

Products of the theoretical effort will be: giant planet spectra, effective temperatures and radii vs. time, predictions for terrestrial planet spectra as a function of planetary system configurations and conditions in which they are embedded, new designs for platforms to detect and characterize giant planets and terrestrial planets.

The products of the earthshine studies will be learning how to interpret low-resolution noisy spectra of an earth-like planet. We expect in the process to generalize these results to planets that are much less like earth.

4. Management Plan:

The management of an Astrobiology Institute node is similar in many respects to that of other Interdisciplinary Programs at the UA in that it involves faculty in several departments working on different aspects of the project but needing to interact frequently and efficiently with colleagues. The goal is to ensure proper coordination while maximizing the opportunities for the individual investigators to develop their ideas. The key to success will be communications. With the proper level of information flow and communication, coordination of the diverse science and educational elements will be straightforward. Therefore the main emphasis of the project management efforts will be facilitation and coordination of the numerous individual participants.

4.1 Project Organization

This proposal brings together, in a cooperative effort within the Laplace Center, a wealth of knowledge, experience, and expertise. The figure below describes the organizational structure and key personnel of our team:

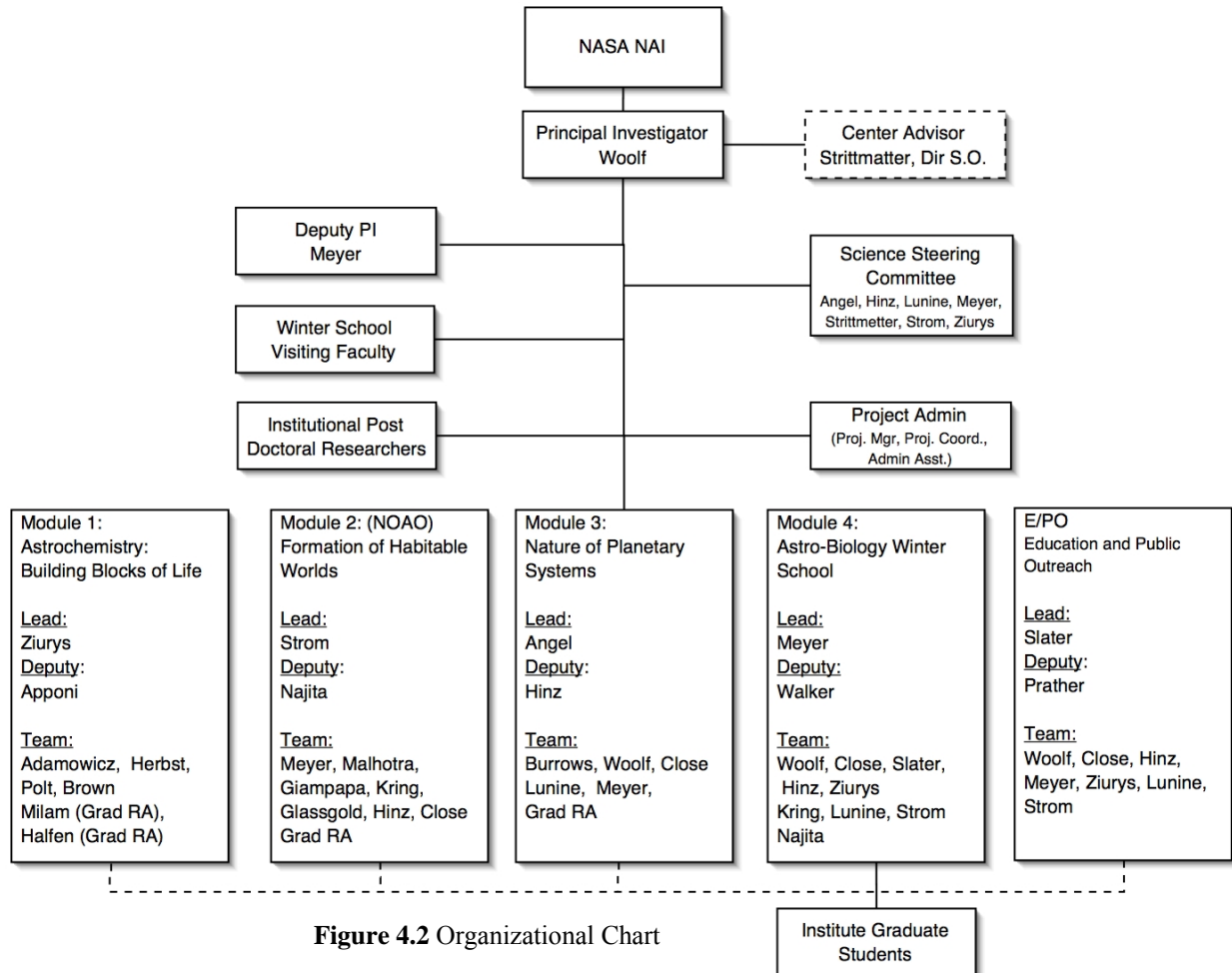


Figure 4.2 Organizational Chart

4.2 Program Management

We propose a strong management structure that will enable us to track the diverse research activities of our collaboration, yet maintain flexibility in allocating resources. The overall responsibility for the effort will fall to the Principal Investigator, Neville Woolf. Professor

Woolf will be the primary arbiter, responsible for the fulfillment of the core science, technical, and programmatic goals. The management team will be augmented by strong Module Leaders who will take responsibility for meeting program objectives within each module. The program management efforts will be led by Thomas McMahon an experienced administrator of major science programs such as the NASA funded, Large Binocular Telescope Interferometer. It is our intension to provide a comprehensive tracking and reporting structure with minimal project cost impact.

4.3 Module Leaders

Lucy Ziurys, Director of the Steward Observatory Radio Observatories, will be the lead for Module #1 focused on astrochemistry. Ziurys will be assisted by Aldo Aponi as her deputy.

Steve Strom, Associate Director for Development for the National Optical Astronomy Observatories, will serve as the leader of Module #2 focused on the formation of habitable planets with Joan Najita as his deputy.

Roger Angel, Director of the Center for Astronomical Adaptive Optics, will be the lead for Module #3 focused on the detection and characterization of extra-solar planetary systems with Phil Hinz as his deputy.

Michael Meyer, Deputy PI, will be the lead for the Astrobiology Winter Institute, which will focus on educating a new generation of scientists in the field of Astrobiology.

Tim Slater, Director of the Science and Mathematics Education Center and Associate Professor of Astronomy will lead the education and public outreach program

Module leaders will be responsible for overseeing the activities of each module, organizing internal team meetings, and providing bi-annual progress reports to the PI. Module leaders will help organize the activities of several members of the contributing scientific staff including faculty, post-doctoral research associates, and graduate students.

As you can see, our program team members are rich with strong institutional and personal heritage in theoretical and experimental astrophysics and astrobiology. This team is well balanced and suited for what we propose.

4.4 Science Steering Committee

A Science Steering Committee will be constituted from the Module leaders and other co-investigators of this proposal. The charter of the committee will be to:

- Assist the PI in the administration of program
- Coordinate the research efforts
- Review and evaluate progress toward the stated science and educational goals
- Facilitate institutional and inter-institutional communications
- Provide a forum for new research paths
- Provide a communications path to other NAIs

The Science Steering Committee will meet quarterly and provide comments, suggestions, and concerns, directly to the Principal Investigator.

4.5 Reporting and Meetings

4.5.1 Monthly Status Meetings

Communications and information management are critical to the success of this program. We plan to hold face-to-face, full team meetings every month for a tightly focused exchange of

information. The agenda will be circulated one week in advanced (advertised throughout the NAI) and honed immediately prior. The Team meetings will be structured to keep team participants informed concerning the wide-ranging activities of the node, but to avoid “meeting-creep”. Our goal is to DO astrobiology, not merely talk about doing astrobiology! At these meetings, Module Leaders will update the team concerning progress toward major milestones (outlined in Figure 4.2). We will encourage team members at other institutions, as well as members of other NAI nodes to participate via electronic conferencing.

4.5.2 Annual Meetings

We will hold annual team meetings as well as hold a full node meeting at the annual general meeting of the NAI. These meetings will be staggered by six months and take the place of the monthly meetings at those times of the year. The main goal of these meetings will be to review the biannual reports of the Module Leaders, to record difficulties in meeting outstanding milestones, identify possible solutions, and to provide for the mid-course corrections of the main science goals for each module. We will make extensive use of the internet with web sites to disseminate documentation and information to those participants not present for our team meetings. This plan allows for flexibility in re-allocating resources within the baseline plan.

4.5.3 Reporting

The PI will report to the Director of the NAI through annual reports and these reports will be made available to the heads of all participating departments, and the Dean of the College of Science at the University of Arizona, as well as the Director of the National Optical Astronomy Observatories.

4.5.4 External Review Board

We plan to constitute an external review panel made up of:

1. The Dean of the College of Science, Department Head, or Director of NOAO;
2. PI of another NAI node;
3. Senior staff member of the central NAI Ames Institute;
4. Outside expert on Education and Public Outreach.

This panel will be invited to our annual team meeting every other year and will provide a report to the PI and the Director of the NAI.

4.6 Tracking

A significant effort of the management team will be the tracking of project finances as well as programmatic goals and accomplishments. The experienced management team possesses a complete suite of tracking, reporting, and implementations plans that have been developed for other NASA programs. Leveraging the existing infrastructure is how we can maintain a small workforce that is focused and highly effective at project oversight.

4.7 Schedule

As indicated in Figure 4.2, we plan a range of activities throughout the period of performance for this proposal. We have identified key milestones (at the rate of 2-3 per year) for each program element and included those in the chart. While each Module stands alone from the rest in terms of schedule and deliverables (avoiding complex dependencies), results from the individual investigations complement and extend the overall impact of each other creating a whole that is

greater than the sum of its parts. The schedule plan also maintains needed flexibility to deal with mid-course corrections suggested by the science steering committee or oversight board. Our schedule plans for significant accomplishments over the period of performance for this proposal that directly address several specific goals outlined in the revised roadmap for the NAI.

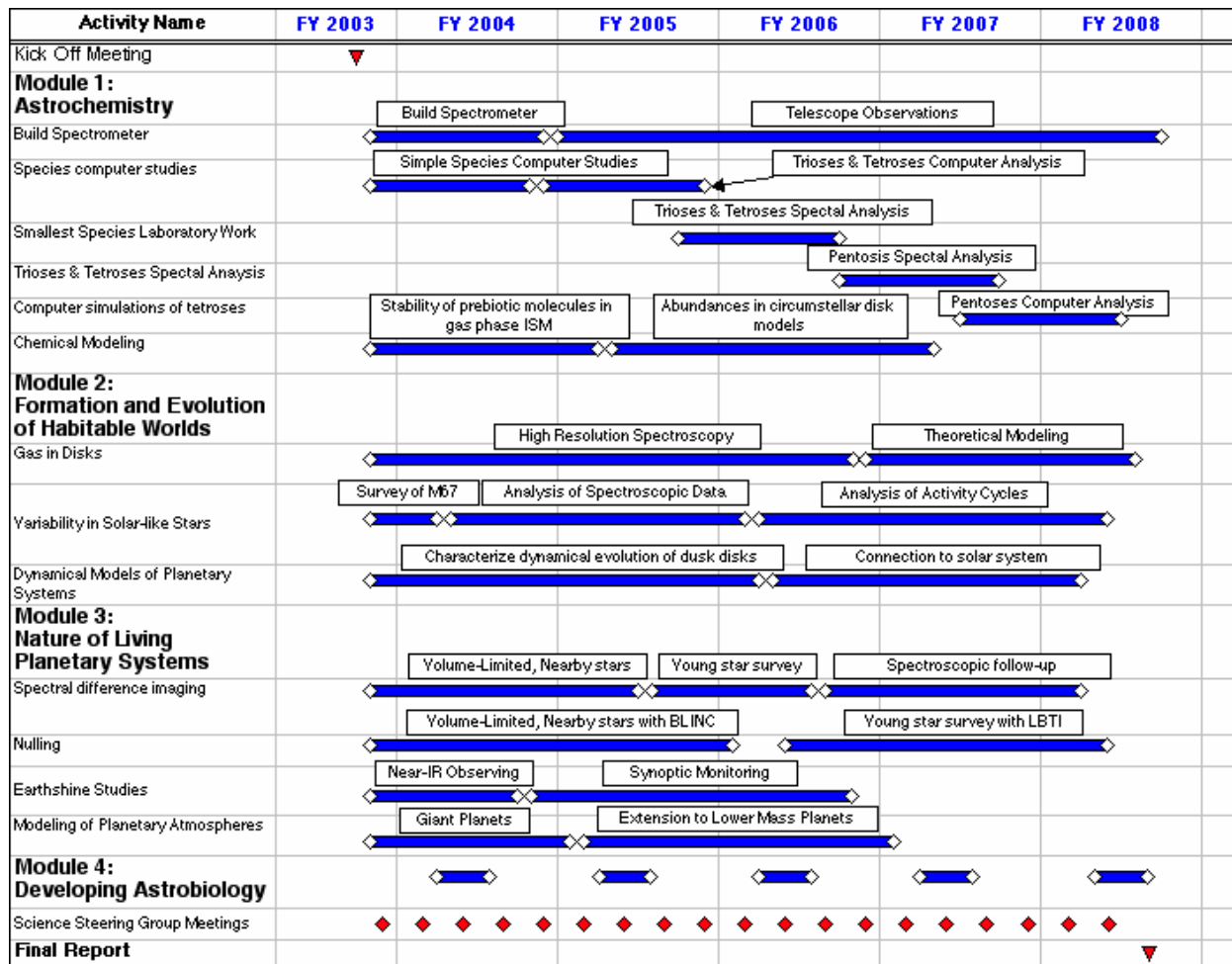


Figure 4.2. Project Schedule

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6.0 Module 4 Developing Astrobiology: Interaction at the Boundaries

Team N. Woolf (Laplace Center, Director), R. Angel, M.Meyer (Winter School, Lead) , P. Strittmatter, S.Strom, L. Ziurys, L. Close, J. Lunine, J. Najita, C. Walker

6.1 Introduction

This module describes how we plan to strengthen astrobiology as an academic discipline and to provide opportunities for students to develop their interests in the field despite the barriers often presented by existing departments. It also contains an educational and public outreach component (EPO).

Despite the fact that the research funding for this proposal is restricted to the work of the three modules, we see a need for a far wider research goal in Tucson. First there are the many astronomical organizations present in Tucson, and a number of them will have their own astrobiology work, which should be coordinated. Then also there is a continuing need, and already activity in interdisciplinary research across the fields of the physical and biological sciences throughout the University of Arizona.

As the National Academy COEL report noted " Astrobiology spans a much larger volume of intellectual and capital resources than the NAI itself. NASA should emphasize the broad base of national scientific capability in astrobiology, ... and not just the institute itself." And there is a need for "enhancing scientific collaborations with non-NAI scientists. To date, NAI has not adequately fostered such collaborations."

At the University of Arizona there are many activities that need to be brought together as part of astrobiology. For example, the Tree-Ring Laboratory has a program in predicting global climate change.(astrobiology goal 6) In biochemistry there is a strong program in organo-metallics that has in the past been used by a different astrobiology node. We need to bring the programs all under a supporting umbrella center to benefit by the interactions.

Only then will we see how to use judicious placement of new faculty hires to fill in key gaps. To achieve our long range goals will take far more than the resources directly discussed in this proposal. It will be necessary to use help wherever it is available. Some help will come from faculty and research associates with alternate funding. Many of them will be in the College of Science at the UA. Some will be in the College of Medicine at UA, and likely other colleges. There will be colleagues outside UA, as for example the NOAO. It will be necessary to meet with many research workers and create an inventory of people resources. It will also be necessary to create an inventory of monetary resources, both for research and teaching. We expect that private fundraising will be required.

6.2 The Laplace Center

Our goals are for the Laplace Center to be the focus of an Interdisciplinary Program (IDP) at the University of Arizona. It will be run by a Director (initially Woolf) and will provide coordination of the entire Astrobiology node (NAI and non NAI work) in Tucson. Members of the IDP will initially be drawn mainly from the current departments of Astronomy, Chemistry (and Biochemistry), Planetary Sciences and from NOAO; it will be open to faculty members from other departments, and there will be an active attempt to recruit them. The UA has a successful

record in multi-departmental, multi-college IDPs, including those in Applied Mathematics and in Neurosciences. IDP programs of study will be developed so that students can earn academic qualifications within the IDP including minors in any of the departmental specializations or vice-versa. The initial focus will be on departments within the College of Science and the Winter School. As opportunity arises, other activity that belongs with astrobiology will be incorporated.

If there are people to do the work, and the needed funds are available we will incorporate the work in the center. If the work seems worthwhile, but the needed resources are not available, the center will try to help find funds. It will develop an inventory of resources. If good research workers are available, and are doing work that fills in gaps, we will try to find employment niches for them. We shall deliberately seek to bring in new faculty members responsive to astrobiology. If the work is astrobiological, the Laplace Center will try to help it.

Fund raising activities will probably be needed. There are possibilities of working with foundations and those who have available money and special interest in astrobiology. The most obvious needs are to find additional funds for outreach, research beyond that funded by NAI and for scholarships for academically deserving students, both graduate and undergraduate. It is clear that current fund-raising activities at UA have not yet tapped the potential for supporting science.

The Laplace Center will also coordinate interchange of faculty with other members of the NAI to develop understanding of issues in all areas of the roadmap. Some of this interchange will be focused on the Winter School, which will also be coordinated by the Laplace Center. Students will not only participate in formal class work and seminars on astrobiology, but will be actively involved in both the astronomical, instrumental and laboratory activities.

6.3 The Winter School

A novel and major item in our proposal is the development of a Winter Astrobiology School at the UA, where we would for one complete semester each year train 20 graduate students (10 from outside the UA) in astrobiology. The Winter School will be organized by Meyer (Deputy PI) with assistance from C. Walker who has experience in developing courses on life in the universe and interdisciplinary graduate programs. His participation will be supported as part of his normal teaching load through the department of Astronomy. We would also bring in visiting faculty to complement our local expertise, especially in areas such as molecular biology of organic molecules, the physical chemistry of life, and artificial and model life, where we do not have enough internal breadth. Over the five years of this proposal we would train 100 students, and make significant strides to develop a broad astrobiology program at the UA and to provide well-trained scientists for astrobiology endeavors at other institutions.

The goals of the winter school are to have two graduate courses for credit that last the complete winter semester. The courses will be broad reaching across the boundaries in astrobiology. Typically there would be one course that was focused on areas of astronomy and planetary sciences which covered origins astronomy and the search for life and a second course which covered molecular biology, fossil and genetic evidence and the origin of life. Meyer and Kring have already developed an interdisciplinary course on the origin of stars and planetary systems.

It is planned to offer 10 scholarships to the best U.S. graduate students who wish to come from outside UA. They would each be given a home in their main discipline. Another 10 students from inside would be admitted, with an initial limit of no more than 3 from any department at UA, and a goal of no more than 2. There would be two to three visiting faculty brought in both to interact with UA faculty, and to help with teaching the second course.

The scholarships would provide travel funds to students from outside UA, homes in departments, and stipends as research/teaching assistants. Credit would be offered for the courses, but the students would be responsible for securing credit (if possible) at their home institution. Every student completing the course satisfactorily would receive a certificate of training in astrobiology.

The logistical sequence will be to arrange for the visiting professors, and securing them accommodations during the previous summer. Also internal faculty roles and lectures will be arranged. Then the opportunities for internal and external graduate students will be advertised in the early fall semester. Applications will be required by the start of October, and students notified of decisions by 1 November. Plans for special experiences, e.g. astronomical observing, geological field trip, biological lab experiences will all need planning during November. External graduate students will be helped to find accommodation during November. Thus the Winter School can start in January without living problems hanging over faculty or students.

Special mentoring will be needed to help students cross the discipline boundaries. The students will be divided into groups of ~5 with moderately common background. Mentoring will need to be done by a professor in the discipline new to them. The student groups will also need help and encouragement from within their discipline.

Each year at the end of the Winter School, the faculty and students will be asked to evaluate the process and suggest modifications. The faculty will then plan for the next Winter School, with the collected evaluation results of the suite of previous Winter Schools to develop revisions to the plan.

6.4 NAI Astronomy Focus group meetings

The first meeting of a potential astronomy focus group occurred at the NAI meeting this spring. We propose to help develop an annual meeting for this group. We suggest alternating annual meetings between the Winter meeting of the American Astronomical Society, and a purely focus group meeting here in Tucson. This would allow both an opportunity for proselytizing among AAS members, and on alternate years to be more focussed towards cross-disciplinary topics. We will suggest that other discipline centered focus groups may do likewise.

6.5 Astrobiology Language and Culture

The study of astrobiology can be seen as the culmination of the process of uniting all the sciences. The great gulf between physical sciences and life sciences started to fill in with the development of molecular biology, but still the parts are held apart by lack of a compelling theory for the initiation of life on Earth, and a demonstration of the existence of life beyond earth. This is the role of astrobiology.

Yet it is hard to change a culture. To move astronomy towards biology, it has to forget its emphasis on great distances, large sizes, huge luminosity and symbolic mathematical demonstrations etc. It needs to return to the idea that the original purpose of astronomy was to find the place and role of humans in the universe. To move biology towards astronomy, it has to remove the emphasis on classification within a system that excludes objects and systems without nucleic acids. It has to focus on the need to put life into a context. The very difficulty of developing a definition of life - the problem in separating the living from crystals and fire is a sign that there is no absolute boundary. Life and the non-living are a continuum, and at present that continuum is extended through other disciplines, but with huge gaps that relate to the origin of life.

Then there is the problem of language itself. At the 1997 International Origins conference in Estes Park, communication between disciplines was at low ebb. There were a series of talks about astronomy, where astronomers only talked jargon to astronomers, ignoring that people from other disciplines were present, totally ignoring the problems of communicating with biologists. And the talks ended with a discussion by a molecular biologist of variations in the form of ATP-ase and discussions about its origin that were totally obscure to all astronomers present, most of whom had not even heard of ATP! Somehow jargon must be discarded where possible and accepted across the board where it is essential, as with ATP. The barriers must be crossed, not only for students entering the field, but also for the benefit of practitioners. Hopefully the process can be worked through in face-to-face meetings, and that is a special strength in developing a broad program in one place. Across-distance communication is, at this time, more likely to end in long unintelligible monologues.

This is a significant issue for NAI's goal to be a virtual institute. There are limits to remote communication at the best of times, probably from the loss of fine body language indicators. The benefits of working day-to-day and face-to-face with those in other disciplines is that we can hope to find ways of presenting material to each other that works, and can be carried into the virtual institute. We hear that astrobiology students at U. Washington developed their own glossary. Perhaps that could act as a cross-disciplinary starting point.

To change the culture of disciplines will also require us to build new habits of meetings, new habits of whom we talk to and how we talk, new habits of how we evaluate research and teaching. Every step will need careful planning and timing, and reflection on the results. Every step will need communication so that people do not feel left out. And regardless of how we do it all, there will be hard feelings of those who feel that they belong to the old way that things were done, and they will resist the change. Nonetheless it is essential to proceed with this development, and the spirit of the time will support the activity.

6.6 Communication Aspects of the Virtual Institute

We see the process of interacting with others at a distance as a two-fold issue. First there is helping NAI with its goals of using visual image communication to be a virtual institute. There is to be a sharing of talks, and an increased interaction in meetings of people who are physically apart. We will help that.

But we also see the benefit of face-to-face interaction. We plan to send our research workers out to other NAI centers and to organizations that are not centers. And we plan to bring in visiting professors, both for our Astrobiology Winter School, and for seminars. And we need to arrange the seminars so that they are spread among the science buildings on campus so that we get all groups into the habit of crossing the ground between the buildings.

One tool that we have tried in astronomy, and which works is an *Annual Internal Symposium*, where we can expose all of us to the broad range of astrobiological work already proceeding in Tucson. During the Winter School there will be a Tucson Astrobiology Internal Symposium, with talks and poster papers. Even the discovery of all the ongoing relevant work will require the help of a number of deans and department heads, so that we can invite all appropriate people to talk and listen

6.7 Advanced Education

6.7.1 Astrobiology Graduate Minors

At the present time we do not see an advanced degree major as appropriate in Astrobiology. Every worker in the field needs a strong background in at least one of the current disciplines. We do however need a graduate minor for future workers in the field. The requirements for a graduate minor in the various departments in the College of Science currently need coordinating. It should be possible for a graduate student in any of the disciplines to get an astrobiology minor by taking appropriate courses that are agreed between the departments. As stated above the IDP will arrange for astrobiology minors to be generally available.

6.7.2 Advanced Undergraduates

Those undergraduates considering going to graduate school to become astrobiologists will be permitted to attend the internal symposium in their final two years. Students in their Junior and Senior year with grade point average above 3.5 will also at their request be assigned a mentor to meet with them at ~ 2 week intervals to discuss their work, encourage their reading, alert them to interesting talks, and generally give them advice and encouragement.

We consider that, at the present time, the best preparation for astrobiology is a strong focus in one of the disciplines that make up the field. Thus astrobiology courses for advanced undergraduates are not recommended at this time. The faculty that plans Winter School will reconsider that issue as we get more experience of the courses and students.

6.7.3 General Education for undergraduates

We will ensure that astrobiology components are available in the UA General Education programs in Natural Sciences—that is science for non-specialists. Astrobiology is a good topic for capturing interest as a general science education topic for undergraduate students in non-science fields. Much of the student enrollment Natural Sciences is in the Astronomy and Planetary Sciences departments, which together provide instruction for over 1,500 students per semester. The Laplace Center will ensure that suitable astrobiology materials are available for these and similar courses in Geosciences, the Tree Ring Lab, Ecology and Evolutionary Biology.

6.7.4 Public Activities

There are many professional astronomers in Tucson and they provide talks at the Steward Observatory Public evenings every month. And there are student and public groups such as the Students for the Exploration and Development of Space, and the Tucson Amateur Astronomical Society where talks, and assistance would be very welcome. The Laplace Center will keep a list of public speakers for astrobiology talks. There are also opportunities for programs on local radio and television, including both public television and radio stations in Tucson.

6.8 Summary

Our goals are to develop a very broad astrobiology research center in Tucson for which the NAI program becomes the initiating momentum. The work will have a focus at the Laplace Center. This will also become the center for teaching and outreach activities. The priority will be focussed on the research because the research is the process that energizes the teaching and outreach.

We see the language and culture barriers between disciplines as major difficulties and will try to break them down with frequent face to face meetings. We believe this will allow us to be helpful to the whole virtual Institute.

The Laplace Center will be started as a UA Interdisciplinary Program (IDP). It will be the focal center for organizing research and teaching, and a cross discipline and department communication center. We will develop a broadly based research program, beyond the boundaries of the NAI sponsored research. We will develop an inventory of local people and monetary resources. We will explore fund raising opportunities.

We propose to hold a biennial NAI astronomy focus group meeting in Tucson, with alternate year meetings at the American Astronomical Society winter meeting. We will also encourage other disciplines to have similar meetings.

Graduate teaching will be focused on an Astrobiology Winter School where two courses will be offered, and ~ 10 graduate students for outside UA given scholarships each year so that they can attend. There are already graduate minor programs in astrobiology in some departments and we will seek to expand this option.

Advanced undergraduates (gpa >3.5) will be allowed to audit the internal symposium, and will be mentored, but we recommend development of competence in one discipline first. We already have a non major general education course offering, and will expand it in so far as demand requires.

6.9 Education and Public Outreach

Team T. Slater (Lead), E. Prather (Deputy), N. Woolf, L. Close, P. Hinz, M. Meyer, L. Ziurys, J. Lunine, S. Strom

A particularly innovative part of this proposed project is for a significant and integrated education and public outreach component. EPO Lead T.F. Slater's primary area of scholarship is the teaching and learning of astronomy. He is the director of the UA Science and Mathematics Education Center and an associate professor of astronomy at UA. His astronomy education research group focuses on identifying students' misconceptions in astronomy and designing effective instructional materials to improve student understanding, both in formal courses and for museums and informal science centers. This unique research group has earned national recognition in the area of astrobiology education by conducting seminal research that systematically studying student beliefs and reasoning difficulties regarding the search for life in the universe (viz. Offerdahl, Prather, and Slater, 2002). This work serves as the foundation for a new laboratory activities manual for undergraduate astrobiology courses for non-science majors (Prather, Offerdahl, and Slater, 2002).

Because a comprehensive program to improve the public's understanding of the this interdisciplinary science requires targeting schools, this research group works directly with secondary school teachers on improving their understanding of the myriad of underlying concepts surrounding the search for other worlds. Through the support of a NSF teacher enhancement award, they have worked with nearly 100 high schoolteachers over the last four summers at the Toward Other Planetary Systems Teacher Leadership Workshop, conducted in Waimea, Hawaii (Meech, Slater, Mattei, and Kadooka, 1999). In addition, to providing numerous workshops at professional conferences for teachers, a NASA education award supports the development and delivery of an Internet-delivered, distance learning course, Astrobiology for Teachers, that more than 100 teachers have already successfully completed (Prather and Slater, 2002). This distance-learning course now constitutes one of the foundational courses provided by the National Science Teachers Association (NSTA) Professional Development Institute. Taken together, a basic research program along side a comprehensive teacher education program uniquely positions this research group to make meaningful and innovative contributions to the present proposal.

Doctoral candidates supported by this program will work on three efforts in the area of education and public outreach. The first effort is to conduct systematic studies of the understanding and beliefs about the scientific search for other worlds held by K-14 students, teachers, and the general public. In addition to contributing to the scholarly literature base of science education, a detailed understanding the existing notions and attitudes people have about this interdisciplinary science are crucial to designing the most effective education and public outreach programs. This will be accomplished through a systematic series of surveys, interviews, and carefully monitored instructional interventions. The results will be disseminated through journal articles and presentations at professional education conferences.

The second effort is to help other graduate students and university faculty supported by this program to become informed about the reasoning difficulties K-12 students, teachers, and the general public have with understanding the search for other worlds. If research scientists have an appreciation for the specific parts of this science that people find difficult, they will be better able to communicate the exciting results and enhance the public's attitudes toward supporting this endeavor. This will be accomplished by conducting frequent workshops and contributing scholarly papers at professional science conferences, as well as regularly

contributing to the program's seminar series. In support of these efforts, the team will undertake the creation and dissemination of an astrobiology public speakers toolkit and a dynamic FAQ (frequently asked questions) on the World Wide Web.

The fourth effort is to provide professional development programming to secondary teachers across the country in implementing high quality curriculum materials that support the interdisciplinary themes and aims of astrobiology. In particular, NAI consortium supported curricula materials that have national appeal and infrastructure, such as the Voyages Through Time Interdisciplinary Science Curriculum. This institute's EPO team is uniquely qualified and positioned to engage and succeed in such a national effort because of their extensive experience in teacher training and their scholarly track record in education and public outreach.

Taken together, these efforts will result in the following as part of the education and public outreach plan:

Referred publications and conference proceedings that contribute to the science education literature base;

Effective analogies and instructional strategies participating scientists can use to help the general public understand and value the search for other worlds; and a better

Appreciation by scientists of the importance of their being actively involved education and public outreach endeavors.

Most importantly, these collective efforts will benefit all community members of the National Astrobiology Institute consortium

In addition to scholarly work in the area of astrobiology educational research and innovative curriculum development, this project supports the scientific research efforts of graduate students working in support of the overall scientific goals described at the beginning of this proposal. As in many institutions, the education of graduate students working along sidepost-doctoral fellows, researchers, and professors is a fundamental and integral part of this proposed project. These doctoral students will pursue newly approved minors at the University of Arizona in biology, chemistry, and planetary sciences, which directly align with and support the overarching themes of this proposal.

Dr. Slater is also working with Discovery Park, a science education center located in Safford, Arizona at the foot of Mt. Graham. His goal is to use the center and the proximity of major astronomical facilities on Mt. Graham to extend the outreach program to parts of rural Arizona and to the San Carlos Indian reservation. The Laplace Center will provide material and support to these efforts.

In addition Dr. Don McCarthy has, for many years, run a very successful Astronomy Camp for high school and university students as well as for teachers using the astronomical facilities on Mt. Lemmon and incorporating components of geosciences and tree ring studies as well as

astronomy. If selected, the Laplace Center will seek to expand this activity and to ensure that suitable materials on astrobiology are available for each of the above program elements.

6.10 References

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