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CONTENTS

Pluto
- A Scientific Wonderland

Dr. Alan Stern, *PI, New Horizons*

Congratulations on the inaugural issue of the letters of the Astrochemistry Society of India! Your journal is appearing at the very time of the historic flyby of the Pluto system, which itself is completing the initial era of the reconnaissance of the Solar System begun with the Mariner missions to Mars and Venus in the early 1960s.

The New Horizons team.

Pluto and its system of moons are the farthest worlds ever explored, and they represent a scientific wonderland. Much of the interest in the system is driven by the composition and chemistry. Today, as I write these words, it is known that Pluto's density indicates a primarily rocky body, with perhaps 35 percentage ice by mass; Pluto's large moon Charon is less dense and contains about equal proportions of rock and water ice. Pluto's surface is covered in super-volatiles like N_2, CO, and CH_4; Charon's, by contrast, is covered in H_2O ice and ammonium hydrates. Pluto has an atmosphere which is also known to consist of N_2, CO, and CH_4, derived from sublimation of the surface ices. We expect to find a wide variety of higher hydrocarbons and nitriles on Plutos surface and in its atmosphere, created by radiation chemistry, photochemistry, and chemical kinetics. We may also find evidence of interesting chemistry taking place now or in the ancient past inside Pluto and Charon.

Just as you launch your journal on 14 July 2015, we expect to be launching a new era in the study of the Pluto system, christened by the data that New Horizons will send back to Earth. On behalf of our mission team, I wish you success in the venture of a new journal, and all the science it reports. I am sure many important communications of research results will grace its pages, perhaps one day even including some results regarding the binary planet Pluto and its moons.

The Molecular Universe

Prof. Alexander Tielens, *Leiden University, The Netherlands*

Over the last 20 years, we have discovered that we live in a molecular universe: a universe where molecules are abundant and widespread; a universe with a rich organic inventory particularly in regions of star and planet formation; a universe where the formation of stars and the evolution of galaxies is driven in many ways by the presence of molecules; a universe where pre-biotic interstellar molecules may represent the first steps toward life; a universe where molecules can be used as dye to trace important processes in the interstellar medium; a universe where molecules provide unique information on the physical conditions of a wide variety of regions; and a universe where molecules can work together to form such complex species as you and me.

Astrochemistry is the study of the organic inventory in space, of the processes controlling molecular formation and destruction, and of the role these molecules play in the evolution of planets, stars, and galaxies. *Astrochemistry is a highly interdisciplinary field and no single scientists can overview all aspects. Progress in our understanding of the Universe is therefore ultimately dependent on how well astronomers work together with chemists, spectroscopists, molecular physicists, and (astro)biologists.* Over the last 10 years, the field has organized itself through networks the European networks, the molecular Universe and LASSIE, the French network Programme National de Physique et Chimie du Milieu Interstellaire (PCMI), the Dutch Astrochemistry Network (DAN) in the Netherlands and the COST networks The Chemical Cosmos, our Astrochemical History and Origins and evolution of life on Earth and in the Universe and through subdivisions of professional organizations the Astrochemistry subdivision of the American Chemical Society and the Laboratory Astrophysics division of the American Astronomical Society. In addition, Elsevier Publishing Company has launched a new journal, Molecular Astrophysics, where researchers working in planetary and exoplanetary science, astrochemistry, astrobiology, spectroscopy, physical chemistry and chemical physics can meet and exchange their ideas. The Astrochemistry Letters launched today at the occasion of the arrival of the New Horizons mission at Pluto fits well in these efforts. This Astrochemistry Letters will serve the needs of the Astrochemistry community by offering a forum for quick exchanges of news, meetings, and ideas in the field of Astrochemistry.

Astrochemistry and Space Astronomy

Dr. S. Seetha, *Space Science Office, ISRO*

Humans have always wondered about the formation of universe as we observe it today and the conditions leading to the origin of life Astrochemistry defined concisely is the study of Chemistry in space environment. It includes observational, laboratory and theoretical studies conducted to understand and detect the formation of elements and molecules and also understand the conditions under which they form and remain stable. Space offers conditions of very low temperature and pressure, difficult to recreate on ground. These conditions enable formation of some molecules which may not be possible under earth like conditions.

Hydrogen is the most abundant element in space. Most of the other higher atomic mass elements that we observe around us are formed in the interiors of stars. The interiors of stars have very high temperature and pressure and these conditions determine which of the nuclear reactions will take place to give the abundance observed in stars. Spectroscopic techniques have enabled the discovery of these elements. These reactions can only be studied in astronomical context as we have still not been able to simulate such conditions for fusion in laboratories on Earth. In fact the final proof that indeed the nuclear reactions are occurring as predicted by models have been possible by detection and solution of the solar neutrino problem. The discovery of elemental lines both from surface of stars and interstellar and intergalactic matter have been through optical and radio astronomy, using advanced ground based telescopes. The interiors of the stars in fact are directly observed only towards the end stages of their life when they expel all their outer layers and lay bare their inner layers ending their phase of nuclear fusion and evolving into compact objects like white dwarfs or neutron stars. With high resolution capabilities of the IUE satellite in UV and sophisticated spectroscopic capabilities of the CHANDRA and XMM-NEWTON telescopes operating in the X-ray band, the interiors of the stars have indeed been observed in planetary nebulae, supernovae and their remnants. Other techniques like asteroseismology also provide information on the cores of white dwarfs and their constitution.

While all these studies are mainly on elemental abundance, interstellar matter with their sparseness provide evidence of molecules which have been observed primarily through radio techniques and in recent years with advanced detection techniques in Infra-red and submillimeter wavebands including the SPITZER satellite mission and Atacama Large Millimeter/sub-millimeter array (ALMA). These consist of inorganic and organic molecules including polycyclic aromatic hydrocarbons(PAHs) which can lead to DNA. These have led to great strides in the area of astrochemistry to understand the conditions leading to the formation of these molecules. Recently the sugar molecule glycolaldehyde has been discovered which is required for the formation of ribonucleic acid (RNA).

Thus it appears that stars spew forth elementary matter at the end of their evolution, molecular clouds can play a crucial role in star formation thus completing the cycle. It may be mentioned that many of the hydrocarbons discovered in interstellar matter are also found in cometary ices. The STARDUST mission has been so far the most sophisticated with detailed studies from cometary constitution.

With these detections modeling of interaction under space conditions and calculations of reaction rates now form a crucial part of research under astrochemistry.

Further, the discovery of dust rings around stars and that of over 1000 exoplanets, the time is now ripe to apply astrochemistry techniques to the interaction of gas and dust and formation of planets and explore whether molecules are formed well before the planets are formed. With this the connection of astrochemistry and astrobiology can be established as to which chemical building blocks can lead to the formation of life even in its elementary forms.

The Indian Space Research Organisation has now undertaken several initiatives towards space exploration. It began with the Chandrayaan-1 mission through which the existence of water on moon was confirmed. This is followed with the presently ongoing Mars Orbiter mission which is providing data on the Mars surface geology and its atmosphere. ISRO plans to have a roadmap for further planetary exploration. One aspect of this will definitely be exploration for chemical constituents in the atmosphere and also on the surface of planets. *'With the coming together of astrochemists and probably also astrobiologists in the country, it is necessary that this group propose and undertake new experiments to be flown on future Indian planetary missions.'* These could be connected with the study of Astrochemistry within the solar system and also for remote sensing of chemical constituents in exoplanets. This would extend the research capabilities within the country from the present geological and atmospheric studies of planets to chemical and biological studies which could lead to new discoveries in these areas of research. Any new findings in terms of observations or modeling in these areas ccan provide a better understanding of the vital question of origins of life.

It is therefore extremely fortunate that we have been witnessing to these recent exciting discoveries and hope that with the advances in astrochemistry will be privileged to view its impact as we are probably on the verge of finding a solution to the origin of life.

VUV Spectroscopy and New Horizons

Prof. Nigel Mason, *The Open University, UK*

The use of spectroscopy to explore planetary atmospheres and planetary surfaces is well established, IR and visible spectroscopy is commonly used to identify atmospheric composition; monitor airglow; categorise ices and minerals on planetary and lunar surfaces and to explore the chemistry on dusty grains in the ISM. However, strangely VUV spectroscopy has been much less used in such studies despite its ability to characterize chemical species and ice morphologies.

The New Horizons mission is about to change this paradigm providing the most detailed VUV spectra of a range of planetary bodies. Aboard the New Horizons mission is the ALICE instrument, an imaging spectrograph designed to perform spectroscopic investigations of planetary atmospheres and surfaces at wavelengths between 520 and 1870 A^0. Using Alice unprecedented VUV images of Pluto and its accompanying moon Charon will be recorded during flyby on July 14, 2015 with the objective of characterizing the neutral atmosphere of Pluto and determining its escape rate and studying the UV reflectance properties of the surfaces of both Pluto and Charon as well as Pluto's other small moons. After its rendezvous with Pluto-Charon New Horizons will continue to explore other Kuiper Belt Objects (KBOs). With Alice measuring their VUV surface reflectance and searching for atmospheres around KBOs.

In order to interpret the data recorded by ALICE laboratory data on VUV ice spectra of potential constituent species and minerals must be recorded. A 'VUV ice catalogue'is being constructed by Dr Bhala Sivaraman and his group in the Physical Research Laboratory, Ahmedabad in collaboration with Professor Nigel Mason and the astrochemistry group at the Open University, UK. Spectra are recorded using VUV light available on synchrotron facilities at Aarhus University, Denmark and Taiwan Light Source. Data is available in a new online database ACID (AstroChemical Ices Database).

VUV Photochemistry of Interstellar Molecules

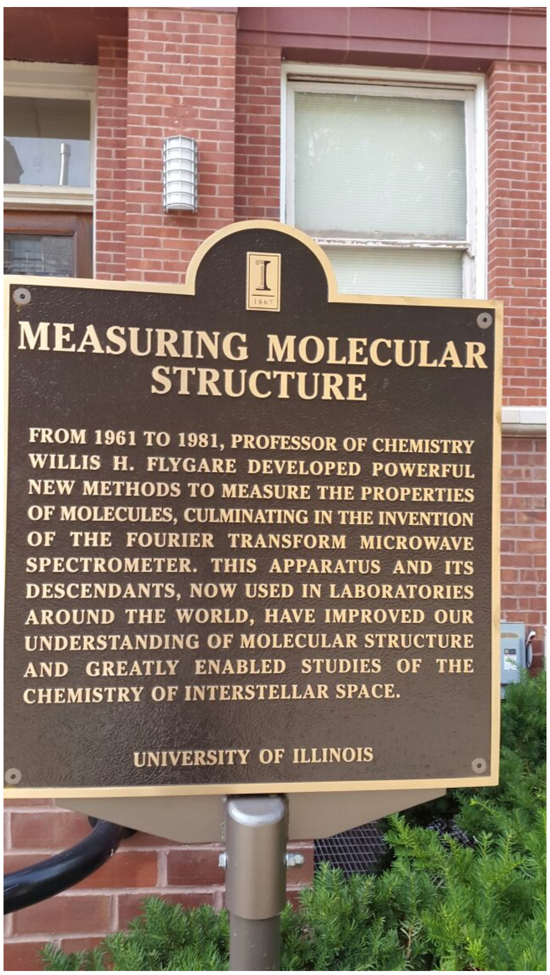
Dr. Bing-Ming Cheng, National Synchrotron Radiation and Research Center, Taiwan

The spectral quality of light emitted from a star depends strongly on its temperature. For example, the maximum intensity of the sun (mean temperature 5778 K of the solarsphere) occurs at about 500 nm and decreases rapidly at wavelengths less than 400 nm. In the region less than 200 nm, solar radiation consists mostly of emission lines, such as H Lyman-at 121.6 nm, superimposed on a rapidly declining continuum; the photon flux from 400 to 700 nm is 10^3 - 10^6 times the flux of the solar continuum in the VUV region. However, the energy of the latter photons, much greater than for visible light, is enough to break any chemical bond of any interstellar molecule. Light of wavelength less than 200 nm might hence be an important driving force for evolution in not only our solar system but also other spatial environments. Investigation of the VUV photochemistry of interstellar molecules is thus intriguing in astroscience; research in this field is currently increasing.

It is important to know which electronic state and what magnitude of the absorbance of the interstellar samples are involved in the VUV photoexcitation processes. For this reason an investigation of the spectroscopy of interstellar molecules in VUV region is urgent and crucial. In cold outer space, molecules may exist in condensed phases; for example, at the temperatures of Pluto, Triton and other trans-Neptunian objects are typically less than 40 K, CO, CH_4, and N_2 occur there in solid forms. The VUV spectroscopy and photochemistry of molecule in condensed phase differ from that of gaseous ones and warrant attention. Our best wish to the success of the Letters of the Astrochemistry Society of India in that it will convene important research results of VUV spectroscopy and photochemistry, that are definitely significant to the advancement of our understanding of the universe.

Astrochemistry and Microwave Spectroscopy

E. Arunan, *Indian Institute of Science, India*



A plaque honouring Prof. Bill Flygare in University of Illinois.

Physics is considered the study of energy and chemistry that of matter. Einstein equated physics and chemistry with his famous equation $E = mc^2$! While atomic physics and molecular physics are standard sub-disciplines in physics, atomic chemistry does not exist. Only when atoms combine to form molecules, liquids, solids etc., we have chemistry. When it came to studies of interstellar molecules, they have so far been grouped under Astrophysics.

I am indeed pleased to learn about the launch of Astrochemistry Society of India. It is quite timely as the American Chemical Society had started the Astrochemistry Division only last year. One might ask, why start Astrochemistry as a new discipline? While such division of science into various disciplines could become arbitrary, often it does help in advancing science. For one thing, there is a dire need for trained chemists to work in problems related to interstellar molecules as our understanding of their origin is still primitive. Understanding the origin of molecules in our universe is important to understand the origin of life! Indeed, astrochemistry as a discipline should perhaps have started decades ago. Better late than never!

Now there are over 200 molecules that have been detected in interstellar and circumstellar space! I have put molecules within quote as these 200 include not only stable molecules such as H_2, CH_3NH_2, CH_3COOH, C_6H_6 and C_{60} but also radicals like CH, C_2 and CH_3CO and ions such as C_8H^- and C_{60}^+.

These radicals and ions would not be considered as molecules by a typical chemist but for 'Astrophysicists', they are listed in Tables of interstellar molecules! The vast majority of these molecules have been detected based on their rotational transitions occurring in microwave/millimeter wave regions. At the ambient temperature in the interstellar medium, rotational excitation is possible whereas vibrational and electronic excitations are beyond reach. Hence, microwave emission is easily detected from interstellar medium.

Indeed, microwave spectroscopy has played a pivotal role in identifying and characterizing interstellar molecules. In particular, the pulsed nozzle Fourier transform microwave spectrometer designed and developed by Bill Flygare at the University of Illinois around 1980 has been crucial. At the Indian Institute of Science, Bangalore our laboratory houses one such home-built spectrometer. Somewhat coincidentally, on 24th June 2015, during the 70th International Symposium on Molecular Spectroscopy, University of Illinois unveiled a plaque honoring Bill Flygare in front of the Noyes Laboratory.

The plaque reads: From 1961-1981, Professor of Chemistry Willis H. Flygare developed powerful new methods culminating in the invention of the Fourier transform microwave spectrometer. This apparatus and its descendants, now used in laboratories around the world, have improved our understanding of molecular structure and greatly enabled studies of *'the chemistry of interstellar space.'* Indeed, the Astrochemistry Society of India is beginning at the right moment. I wish this Society can influence the growth of Astrochemistry in India and the World!

Pluto Analogs - Colder and Closer

Indhu Varatharajan and Bhalamurugan Sivaraman, *Physical Research Laboratory, India*

Few craters in the Lunar north and south poles are in permanent shadow for millions of years, in particular the Shackleton crater. This crater lying in permanent shadow is known to contain layers of molecular ices. Even in one crater the molecular composition varies with respect to the temperature gradient within the crater. Not just our neighbour, even the closest planet to the Sun, Mercury, holds some of the coldest craters that harbor molecular ices. Irrespective of how close we are to the Sun, it is the permanently shadowed regions that can act as shelter and in fact are the cold chemical factories synthesizing the complex molecules.

In PRL, we simulate the conditions that prevail in the coldest craters that are found on our own Moon, icy craters of Mercury, and the icy mantles of cold interstellar dust grains that can reach up to 10 K, and the icy satellites of Jupiter and Saturn, such as Europa and Titan. Even the molecular ices found on long and short period comets are also studied experimentally. Ground based experiments on Martian polar ices are also studied In support of the Indian Mars Orbiter Mission. From the outcome of our ground based experiments simulating the icy bodies of the Solar System, we believe that understanding the icy craters of our own Moon may provide the analogy for deeper understanding of molecular synthesis on colder regions of space, especially, the icy bodies of the outer Solar System. On the occasion of the first encounter of a spacecraft with Pluto we propose that, in fact, these permanently shadowed craters are among the best analogs of such distant icy bodies of the outer Solar System that are well within our reach.

Interestingly, this mysterious world could be studied and understood by exploring the colder parts of the lunar system called the cold traps in the lunar poles. The cold traps are the permanently shadowed regions in the lunar poles those holds the presence of tonnes of ices trapped in them. The sources of these ices are exogenic and the main delivery system could be the comets and icy debris from the Kuiper belt itself. As Pluto resides among these icy comets and debris in this faint disc, the chemistry of these icy cold traps of the Moon as well as Mercury could invariably act as a proxy to the chemistry of the Pluto surface. With the surface made up of a frozen ice of complex organic molecules, the chemistry of the average Pluto surface composition could invariably be similar to the chemistry of the ices in the cold traps of Moon and Mercury.

The in-situ exploration of these ices of the poles of the Moon will help us to bridge the gap between the magnanimous distance between Earth and Pluto. We would like to emphasize that we are not claiming that the cold craters on Lunar poles could explain the entire icy chemistry of outer Solar System bodies. However, we are quite confident that it could indeed explain and contribute to a certain extent on our understanding of the icy bodies of the outer Solar System.

ASTROCHEMISTRY SOCIETY OF INDIA
ESTABLISHED 2015

New Horizons @ PRL

July 14, 2015

Venue: Ground Floor Lecture Hall
Time: 09:30 AM to 04:30 PM

Program Schedule

Telescopic view of Pluto	***Shashikiran Ganesh***
Pluto on paper	***A. K. Singal***
Geology of Pluto	***Amit Basu***
Atmosphere of Pluto	***Smitha Thampi***
Spectroscopy of Pluto	***Raja Sekhar***
Space Instrumentation	***Shyama Narendranath***
New Horizons Vs Rosetta	***Chaitanya Giri***
Analogs and Astrochemistry of Pluto	***Ankan Das/Amit Pathak***
Concluding remarks	***Bhalamurugan Sivaraman***

New Horizons @ PRL

14th July, 2015

Telescopic view of Pluto

Pluto was discovered by Clyde Tombaugh in 1930. At the time of discovery it was thought to be as massive as Jupiter. Soon it was found that it was much smaller than expected. Pluto's orbit is quite different from the rest of the planets and for some part of the time, it is nearer to the Sun than Neptune. After the discovery of other similar sized objects beyond Neptune, it was clear that Pluto was a prototype of similar objects, collectively called Trans-Neptunian Objects - TNOs. In this talk, I shall review the circumstances of Pluto's discovery and some interesting events and discoveries from observations using earth-based and near-earth telescopes. The Pluto system is being visited by New Horizons after a fast paced journey of 9 years through the Solar System. We look forward to the results from this exciting mission to the outer Solar System. These observations will tell us how similar these denizens of the outer solar system are to those that, once in a while, visit us in the form of Kuiper belt comets.

-Dr. Shashikiran Ganesh,

Physical Research Laboratory

Reaching Pluto - A ride on the New Horizons!

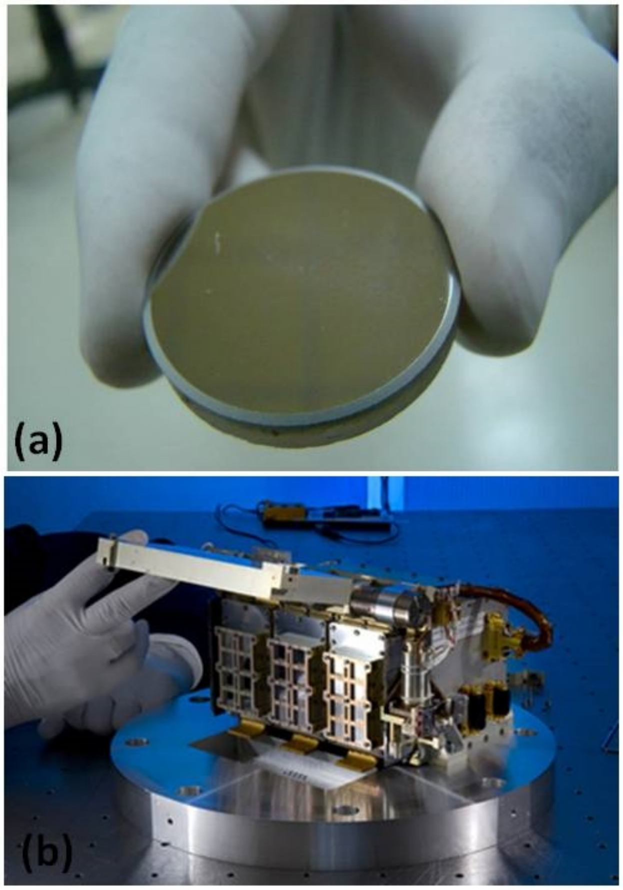
The New Horizons was launched on January 19, 2006, and now after a long journey of about 5 billion km, lasting 9.5 years, is reaching Pluto on 14th July 2015. It is a flyby mission passing within about 12,500 km of Pluto, sending us pictures and data on Pluto and its five moons. New Horizons has the distinction of having the highest ever launch speed of 16.26 kilometers per second (58536 km/h), which is about 40 times the speed of a bullet fired from a revolver.

After a brief encounter with asteroid 132524 APL on its way, New Horizons proceeded to Jupiter, and with the help of the gravity of Jupiter, borrowing a tiny bit of the planets kinetic energy, boost its speed further, which has cut its journey time to Pluto by years. We will discuss how a spacecraft uses a planet's gravity to boost its speed. After Pluto, New Horizons will proceed further to study some possible targets in the Kuiper belt.

-Dr. A.K. Singal,

Physical Research Laboratory

Space Instrumentation for Planetary Chemistry



(a) The x-ray mirror is a new development for imaging X-ray spectroscopy of planets.
(b) C1XS flown on Chandrayaan-1 to study chemistry of the Moon.

All the objects in the Solar System from the giant Jupiter to tiny specks of dust formed billions of years ago in nebula around a young Sun. Yet the chemistry of the planets and small bodies vastly differ. Even Venus, often called Earth's twin though believed to have started off with similar composition has evolved into a completely different environment.

Understanding planetary composition is a crucial element in deciphering the physical and chemical processes these objects have gone through since their formation. With the great success of the first Indian lunar mission Chandrayaan-1 and recently the Mars Orbiter Mission, India has entered the golden age of planetary exploration. As opportunities open up, a most arduous task is to design and develop instrumentation to address the science goals. I will talk about techniques to understand planetary surface composition focusing on X-ray instrumentation on Chandrayaan-1 and 2 as well as for beyond.

-Dr. Shyama Narendranath,

ISRO Satellite Center

Atmosphere of Pluto

The atmosphere of Pluto is dominated by N_2 followed by CH_4 and a trace amount of CO. Plutos eccentric orbit and large obliquity result in significant changes in global and local solar insolation over the course of a Pluto year. Because its nitrogen-dominated atmosphere is supported by vapor pressure above the surface ices, the properties of the atmosphere depend critically on the surface temperature of these ices.

The atmosphere is believed to be extending to heights comparable to its radius and is hydrodynamically escaping. The atmospheric dayglow emissions are expected to be similar to that of Titan. The Pluto has a weak ionosphere and the escaping exospheric neutral atoms get picked up by the solar wind, and this region exhibits a transition from a cold collisional ionosphere to energetic, mass loaded solar wind flow.

The New Horizons flyby of Pluto in July 2015 will be the first visit of a man-made object to Pluto. The New Horizons is carrying several instruments to study the

atmosphere of Pluto. The ALICE spectrograph is aimed at observing Pluto at EUV and FUV wavelengths. This might observe various emissions. The SWAP and the PEPSSI instruments will observe the solar wind and energetic particle populations of Pluto.

The predictions for the New Horizons observations by these instruments about the atmosphere of Pluto will be discussed in this talk.

-Dr.Smitha V.Thampi,

Space Physics Laboratory

Geology of Pluto

The current understanding about the solar system processes of interaction of energy and matter between different systems and sub-systems is based on various theories, which are explained by either direct scientific observations or simulated models based on those observations. These understandings help us to emphasize on some specific objectives of a planetary exploration.

Very little information is available todate about the Geology of Pluto, which not-only resides at the outer fringe of the Solar System but with some unique geological features in comparison to the terrestrial and gaseous planetary bodies posts long-standing queries to the scientific community.

The terrestrial planets are smaller in size with solid surfaces than the gas giants, which all have no solid surface and contain larger number of satellites. The icy-body Pluto is more like a terrestrial planet with small size and solid surface but still resides near the Kuiper belt. Further, the volatile ice content of Pluto is higher than the icy satellites of the gas giants. However, speculations of the geology of Pluto should be made through the analogue observations from the icy satellites of similar size, e.g., Ganymede, Callisto, Europa, Titan, Triton etc; thanks to Voyager, Galileo and Cassini missions.

A variety of endogenic landforms were created by volcanic resurfacing, including cryovolcanics in the form of active outgassing through narrow plumes on the icy satellites, e.g., Triton. These observations are useful to constrain the chemical and thermal evolution of Pluto. Another endogenic process which could have structured the landform of Pluto was the early tectonic activity forming faults, grabens and ridges. These structural features are the imprints of periods of global expansion and contraction due to a heat buildup from radiogenic sources, volcanic diapirism, and periodic phase-changes of ice/water at the interior and on the surface. Pluto also likely to have small and shallow impact craters similar to other icy bodies, as the impactors traveled slower than those on the terrestrial planetary bodies. Pluto has an atmosphere (approx 50 microbar surface pressure) at its perihelion position, triggering aeolian activity that may create landform like dune.

NASA's New Horizons has discovered remarkable geological features on Plutos surface as yet. Those are: (1) an immense Dark band known as the Whale near the equator; (2) an immense bright feature shaped like a heart near the equator; (3) evenly spaced dark spots at the equatorial region stretching approximately 1600 km long in the east-west; and (4) a recently found polygonal feature above the equatorial region. Scientists expect pouring of a wealth of information from the New Horizons'Pluto exploration in coming few days. The new discoveries will tell us about the global geology and geochemistry, which in-

turn will make possible to understand the formation and evolution history of Pluto.

-Dr. Amit Basu,

Physical Research Laboratory

Astrochemistry of Pluto

Like alternative members of the Kuiper belt, Pluto is believed to be a residual planetesimal; a part of the protoplanetary disk round the Sun that did not absolutely coalesce into a full-fledged planet. Pluto offers the rare chance to review a really cold planetary atmosphere that conjointly evolves powerfully with time, and will after all be transient, sinking and freeze out on the surface.

In order to understand the chemical composition of Pluto and find a linkage between the interstellar ice and the ice of Pluto, it is necessary to understand its origin. So, think about a consistent disk model that takes care of the protoplanetary disk structure together with the gas/grain chemistry with correct inclusion of all radiation sources (stellar ultraviolet illumination, X-rays and external) would be a good idea. Coupled region and surface model with all sources of radiation would also be useful to know the alteration of the chemical composition during seasonal changes. Chemical changes of the ice could be due to various charged particles so understanding the properties of these particles (penetration depth, sputtering yields etc.) would be of prime importance. Theoretical model would be developed to study the constituents of the Pluto ices and atmospheres. Quantum chemical calculations would also be used to elucidate the observed spectrum.

-Dr. Ankan Das,

Indian Center for Space Physics

VUV Spectroscopy of Pluto

Please refer to page 5 for the abstract.

Understanding Molecules of Interstellar Relevance by Optical Spectroscopies

Radha Gobinda Bhuin, Indian Institute of Technology Madras, India

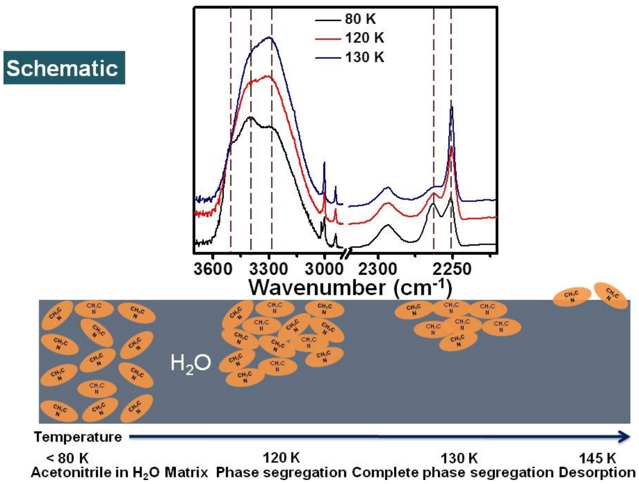
PhD thesis abstract

Different physical and chemical phenomena occurring in molecular solids have diverse implications in various fields ranging from physics, chemistry, materials science to biology. These diverse processes include phase transition, diffusion, dewetting, adsorption, catalysis, molecular recognition, self-organization, chemical transformation, etc. Studies of molecular solids are performed using versatile spectroscopic and spectrometric techniques. Spectroscopic techniques such as infrared (IR) and vacuum ultraviolet (VUV) spectroscopies are important tools to explore the properties of molecular solids. Infrared spectroscopy is an excellent technique to investigate various properties like adsorption, phase transition, interaction, detection of new molecules, etc. VUV spectroscopy provides information about morphology of molecular solids, electronic structure and is useful to identify new molecular species.

In chapter 1, an overview of molecular solids present in the different environments has been depicted with an emphasis on the most abundant molecular solid, water-ice. Molecular structure and different phases of water-ice has been described in details. Various scientific methods which are used to understand molecular solids have also been described briefly. With specific examples, each technique has been demonstrated.

Chapter 2 describes the spectroscopic techniques used to understand molecular solids. The techniques used in here which are RAIRS and VUV have been discussed in more details. Especially the general principle, how it is being measured, instrumentation and the advantages of using the techniques in understanding molecular solids have been described.

Chapter 3 introduces a new method to understand porosity of amorphous solid water through phase transition of diffusive dichloromethane molecules. Dichloromethane thin films deposited on Ru(0001) at low temperatures (80 K) or lower undergo a phase transition at 95 K, manifested by the splitting of its wagging mode at 1265 cm^{-1}, due to factor group splitting. This splitting occurs at relatively higher temperatures (100 K) when amorphous solid water (ASW) is deposited over it, with a significant reduction in intensity of the high wavenumber component (of the split peaks). Control experiments showed that the intensity of the higher wavenumber peak is dependent on the thickness of the water overlayer. It is proposed that diffusion of CH_2Cl_2 into ASW occurs and it crystallizes within the pores of ASW, which increases the transition temperature. However, the dimensions of the CH_2Cl_2 crystallites get smaller with increasing thickness of ASW with concomitant change in the intensity of the factor-group split peak. Control experiments support this suggestion. We propose that the peak intensities can be correlated with the porosity of the ice film.



Segregation of acetonitrile molecules in water ice matrix as a function of temperature.

In chapter 4, interaction of water-ice and acetonitrile has been studied at low temperatures in their co-deposited mixtures, in ultra-high vacuum conditions. They interact strongly at low temperatures (in the temperature range of 30 - 110 K), which was confirmed from the new features manifested in the reflection absorption infrared spectra of the mixtures. This interaction was attributed to strong hydrogen bonding which weakens upon warming, as the acetonitrile molecules phase segregate from water-ice. Complete phase separation was observed at 130 K prior to desorption of acetonitrile from the water-ice matrix. Such a hydrogen bonded structure is not observed when both the molecular solids are deposited as water on acetonitrile or acetonitrile on water overlayers. A quantitative analysis shows that in the 1:1 co-deposited mixture, more than 50 percent acetonitrile molecules are hydrogen bonded with water-ice at low temperatures (30-110 K).

In chapter 5, following the recent identification of ethanethiol in the interstellar medium (ISM), we have carried out VUV spectroscopic studies of ethanethiol (CH_3CH_2SH) from 10 K onwards until its sublimation in an ultrahigh vacuum chamber, simulating astrochemical conditions. These results are compared with those of methanethiol (CH_3SH), the lower order thiol which is also reported to be present in the ISM. The VUV spectrum of both methanethiol and ethanethiol recorded at 10 K was found to have strong absorption from 107 nm to 210 nm (11.6 to 5.9 eV) with two prominent, broad peaks and a third weak, broad peak. VUV spectra recorded at higher temperature reveal conformational changes in the ice and phase transitions whilst evidence for dimer formation is also presented.

Chapter 6 summarizes the above mentioned results and future perspective of this area of research.

For full thesis please write to radhagobindabhuin@gmail.com

Office of Astronomy for Development

ASTROPROJECT

Documentary Series on Astronomy Research in India

Astroproject is an initiative to develop a Documentary Series on Astronomy, Astrophysics and Space Science related research in India. The project received sanction from the International Astronomical Union Office of Astronomy for Development (OAD). The Project concerns with documenting the Astronomy, Astrophysics and Space Science Research Institutions along with their facilities across the Country. The discoveries and research carried out by the scientists in these institutions are guiding us in revealing several mysteries of the universe. These contributions specifically needs to be highlighted among the students across the educational institutions in India.

The Documentary series shall also highlight the evolution of astronomy in India and also emphasise the importance of research in the field of astronomy. . The documentary series shall be screened in Schools, Colleges and Universities across India and would be done with the help of several stake holders like Research Institutions, Educational Institutes, Universities, Government bodies, Non Profit Organizations and Amateur Astronomy clubs. The documentary series shall also be made available for free download.

We look forward for your active participation in communicating Astronomy and Space Sciences across the country

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Logo description

Astrochemistry Society of India

"Astrochemistry is a highly interdisciplinary field and no single scientists can overview all aspects. Progress in our understanding of the Universe is therefore ultimately dependent on how well astronomers work together with chemists, spectroscopists, molecular physicists, and (astro)biologists..."

Prof. Alexander Tielens

ASTROCHEMISTRY SOCIETY OF INDIA
ESTABLISHED 2015

The logo depicts deep space, simulated in a vacuum chamber, implying that both observations and experiments are imperative in Astrochemistry. The image inside the flange of the vacuum chamber is an RGB colour composite of the M16 (Eagle nebula) region observed with the 50cm telescope at Mt. Abu IR Observatory.

Concept	**Design**	**M16 colour composite image**
S.Pavithraa	*Chaitanya Giri* *(including cover page)*	*Shivali Verma*

Invitation for Submitting Letters

For the next issue on 13th August, 2015

We are pleased to invite your articles (in the form of a 2-3 paragraphs and an image if possible) for the next issue which is aimed to release on 13th August, 2015 on the event of perihelion approach of Comet 67P/Churyumov-Gerasimenko escorted by the Rosetta spacecraft!

Kindly email your articles to acsi@prl.res.in

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