**European Cooperation
in the field of Scientific
and Technical Research
- COST -**

Secretariat

Brussels, 11 December 2008

COST 253/08

MEMORENDUM OF UNDERSTANDING

Subject :	Memorandum of Understanding for the implementation of a European Concerted Research Action designated as COST Action CM0805: The chemical cosmos; understanding chemistry in astronomical environments

Delegations will find attached the Memorandum of Understanding for COST Action CM0805 as approved by the COST Committee of Senior Officials (CSO) at its 172nd meeting on 24-25 November 2008.

MEMORANDUM OF UNDERSTANDING

For the implementation of a European Concerted Research Action designated as

COST Action CM0805

THE CHEMICAL COSMOS; UNDERSTANDING CHEMISTRY IN ASTRONOMICAL ENVIRONMENTS

The Parties to this Memorandum of Understanding, declaring their common intention to participate in the concerted Action referred to above and described in the technical Annex to the Memorandum, have reached the following understanding:

1. The Action will be carried out in accordance with the provisions of document COST 270/07 “Rules and Procedures for Implementing COST Actions”, or in any new document amending or replacing it, the contents of which the Parties are fully aware of.

2. The main objective of this Action is to study chemical processes relevant to the physical conditions encountered in the interstellar medium, and on the surface and in the atmospheres of planetary bodies.
3. The economic dimension of the activities carried out under the Action has been estimated, on the basis of information available during the planning of the Action, at EUR 80 million in 2008 prices.
4. The Memorandum of Understanding will take effect on being accepted by at least five Parties.
5. The Memorandum of Understanding will remain in force for a period of 4 years, calculated from the date of the first meeting of the Management Committee, unless the duration of the Action is modified according to the provisions of Chapter V of the document referred to in Point 1 above.

A. ABSTRACT AND KEYWORDS

Understanding the chemical evolution of the Universe requires a detailed knowledge of the complex chemistry occurring in both the present and past history of the Universe. Such astrochemistry is distinct from that occurring in terrestrial and industrial environments and requires a multidisciplinary approach, bringing together researchers from astronomy, quantum physics/chemistry, surface science, condensed matter physics, nanotechnology, low temperature physics as well as physical chemistry, chemical physics and aerosol/particulate science. The mechanisms for bringing together such a diverse group of researchers are ideally suited to the goals and mechanisms of a COST Action since, initially, it is vital to provide a forum within which the key questions of astrochemistry can be discussed and an integrated research community established to tackle them through a combination of observation, modelling and laboratory studies. This Action will organise a scientific research programme focused around three key topics:

1. Radical- and ion-induced reactions
2. Heterogeneous chemistry
3. Atmospheric chemistry

combined with the creation of an infrastructure under which European astrochemistry research may be developed. The Action will organise conferences, workshops, scientific exchanges and training events for younger researchers. The Action will also develop links with other relevant research programmes in astronomical and planetary science and engage with the general public and strategy makers.

Keywords: Astrochemistry, physical chemistry, heterogeneous chemistry, planetary atmospheres, planetary science.

B. BACKGROUND

B.1 General background

An understanding of the chemical evolution of the Universe necessarily requires that we gain a detailed knowledge of the complex chemistry occurring in both the present and past history of the Universe. Such astrochemistry is distinct from that occurring in the terrestrial and industrial environments within which traditional chemical studies have been conducted for several reasons:

(i) Due to the low densities encountered in many astronomical regions the time scale of chemical evolution of astronomical objects may be tens of thousands (or even millions) of years.

(ii) The chemistry often takes place at much lower temperatures than those commonly encountered on Earth, emphasizing so-called barrierless chemical reactions.

(iii) Chemical species not commonly found on Earth play a key role in astrochemistry e.g. the molecular ions H_3^+ and HeH^+ both of which are believed to take part in the first chemical reactions to have ever occurred in the history of the Universe.

(iv) Much of the chemistry in heterogeneous chemistry takes place on the surface of micron sized grains. The physical and chemical properties of these grains are more akin to aerosols/particulates that are fundamental to nanotechnology than traditional bulk surface chemistry.

Astrochemistry is therefore a very different type of chemistry to that usually conducted by the chemical community and requires a very different multidisciplinary approach, bringing together researchers from astronomy, quantum physics/chemistry; surface science; condensed matter physics, nanotechnology, low temperature physics as well as physical chemistry, chemical physics and aerosol/particulate science. The mechanisms and methodology for bringing together such a large and diverse group of researchers have, to date, been relatively limited and were often at national level (e.g. the AstroSurf programme in the United Kingdom and a long established programme within the French scientific community) but are ideally suited to the goals and mechanisms of a COST Action since initially it can provide a forum within which the key questions of astrochemistry can be framed/discussed and an integrated research community established to develop the necessary strategy and methodology to tackle them through a combination of observation, modelling and laboratory studies.

Such an astrochemistry initiative is extremely timely. First, recent space born and ground based radio to far-infrared telescopes, many of them European (e.g. ISO IRAM or JCMT) have revolutionised our chemical picture of the Universe providing for the first time chemical maps of the Universe with tantalising hints as to the chemical evolution of the cosmos. These new observations have highlighted our ignorance of many aspects of astrochemistry and dramatically shown the necessity for a new inter-disciplinary approach. Secondly the new European satellite Herschel, planned to be launched in 2009, promises to provide a new space observatory to explore the cosmos over the spectral range from the far infrared to sub-millimetre, which may revolutionise our view of the molecular nature of the Universe. Thirdly, the outstanding success of Mars Express (the first purely European mission to another planet), the dramatic landing of the European Huygens probe on Titan in January 2005 and the on-going success of the European packages on the joint ESA/NASA Cassini-Huygens mission to Saturn have shown Europe’s ability and innovation in space technology. The launch of the Rosetta mission to study and land upon a comet, Europe’s major investment in the European Southern Observatory (ESO), through use of the Very Large Telescope (VLT) and the approaching use of the Atacama Large Millimeter Array (ALMA) and the development of the Darwin Space Telescope array to search for life supporting exo-planets, indicate the breadth and innovation of the European astronomical, planetary and space scientific research community.

B.2 Current state of knowledge

Astrochemistry is broadly defined as the study of chemical reactions under the physical conditions prevalent in astronomical objects, whilst these may range from very hot environment of stars and extreme events such as supernovae to low temperature regions of the interstellar medium (ISM), those vast regions of space between the stars that appear (to the visible eye) to be empty. However, through astronomical observations in the radio and infra red (IR) spectral regions it has been unambiguously established that these regions are in fact enormous chemical factories with over 150 molecules having been observed ranging from the simplest diatomics such as H_2 and CO to polyatomic molecules such as acetic acid, formamide and benzene. Such a rich chemical complexity is seemingly counter intuitive to the laws of chemistry as understood and used on Earth.

The ISM is cold (temperatures of 10-100K) and empty with pressures of less than 10^{-12} torr such that the probability for a collision between two compounds is low and, at such low temperatures, the reaction rate would be expected to be very slow (hence in most industrial chemistry the reactants are heated to increase their reactivity). The solution to this apparent paradox is that the chemistry in the ISM is somewhat different from the conventional chemistry we observe on Earth. The ISM contains several different sources of radiation:

– Light (produced from stars) of which the ultraviolet is the most important for inducing chemistry.
– Cosmic rays (high energy ions) about 89% of which are protons, 10% helium nuclei (alpha particles) and about 1% ions of the heavier elements. It is believed that most galactic cosmic rays derive their energy from supernova explosions, which occur approximately once every 50 years in our galaxy.

Such radiation sources have sufficient energy to break the chemical bonds of molecules in the ISM and thence produce both reactive radicals and ions capable of inducing further chemistry. In the gas phase much of the chemistry in the ISM is driven by such ion- and radical-induced reactions. Such reactions tend to be barrierless, which implies that if the reactants pass each other within a defined (velocity-dependent) cross section a reaction always occurs. They can therefore occur at low temperatures, indeed in many cases their reaction rate constant actually increases with descending temperatures.

Photo-induced and electron/ion-induced gas phase chemistry is also central to the physical and chemical processing of planetary atmospheres. For example, the aurorae on Earth are caused by magnetospheric interaction with the Earth’s upper atmosphere and similar effects have been seen on Jupiter and Saturn. In such atmospheres many chemical species are formed under unusual chemical conditions; for example the haze that covers Titan is an aerosol formed by polymerisation of cyano compounds generated by photon- and ion-induced chemical processes from methane and nitrogen. However, despite the success of ion-molecule and radical chemistry in explaining some of the molecular formation in the ISM and planetary atmospheres, many of the molecules formed and the time scales upon which they develop can not be explained by gas phase reactions alone. For example, for molecular hydrogen (the most abundant molecule in the ISM) there is no gas phase reaction scheme that can explain its formation.

Thus it is necessary to consider the role of the dust in the ISM. Dust comprises about 1% of the mass of the material in the ISM and can act as a surface upon which chemistry happens. The dust is mostly carbonaceous or silicate in nature, comprising of small particles, typically sub-microns in size, probably with an irregular (perhaps fractal) structure. Being extremely cold (around 10K) the dust grains act as a depository for any gaseous molecules, which stick to the surface. Hence H atoms may be trapped on the surface and subsequent reactions between such H atoms are now believed to be the main mechanism by which molecular hydrogen is formed in the ISM. The product H_2 is then desorbed back into the ISM most likely by the heat of formation released during its creation.

Other gaseous atomic and molecular species in the ISM may also collide with the dust slowly forming a complex multi-component ice layer. It is this ice that provides the high density target within which chemistry may be induced by interstellar radiation allowing more complex molecules to be formed. Similarly, most of the planetary and lunar surfaces in our own solar system (Venus and Mercury being the exceptions) contain large amounts of ice. Most of the outer Solar System bodies are covered in ices, as are a number of the satellites of Jupiter and Saturn. In particular, Europa has recently been studied in detail to establish whether it is possible for a subsurface ocean to be present and recent evidence for the presence of ozone (previously thought to be characteristic of bioactivity) has been reported on Saturn’s moons Rhea, Dione and Enceladus, and the Jovian moon Ganymede. Nor should we forget that the large number of Kuiper belt objects located beyond Neptune, including the recent planetoid object, 2003 UB313, are icy bodies. Similarly cometary systems are mainly comprised of ice. Hence ice is perhaps the most common phase of matter in our own solar system and is likely to be the most common phase in other planetary systems and heterogeneous chemistry must therefore play a vital role in the chemistry of the ISM and planetary science.

B.3 Reasons for the Action

The major rationale for this Action will be to exploit the mechanisms of the COST scheme to define, free of any constraints of a particular agency, national programme or particular space mission, the key scientific questions of modern astrochemistry and to develop a framework within which these can be addressed. Indeed the Action will play a major role in setting the agenda for European astrochemistry research providing a networking structure (the European Astrochemistry Network) that will exist well beyond the four years of the Action, forming with the already established Europlanet (for planetary sciences) and European Astrobiology Network Association (EANA, for astrobiology) partners of choice for the European Space Agency, ESA, when planning its future space and planetary missions. Prior consultations with these bodies have demonstrated their willingness to support this Action both in kind and financial support (towards joint meetings). The Action will also provide a novel and much needed forum for bringing together scientists from disparate fields necessary for conducting the interdisciplinary research characteristic of astrochemistry. Whilst it will not fund basic research the Action will provide opportunities for scientific exchanges which (as demonstrated in other Actions) leads to high quality scientific outputs and establish long term research co-operations between participating research teams. Targeted research topics are listed below.

The Action will also provide a central role in the organisation and dissemination of the myriad of data required for astrochemical studies. Publications of proceedings of topical meetings (organised by the Working Groups) and the Annual Workshop will provide much needed reviews of current research and indicate key areas of future research. The Action may also provide a vital platform for the assembly and development of vitally needed databases for astrochemical research.

The multidisciplinarity of astrochemistry requires training for a new generation of scientists capable to work across the traditional borders of science. The Action will therefore engage in organising interdisciplinary training events in collaboration with existing European institutions and networks.

Finally this Action will have a specific activity directed towards public engagement. Astrochemistry and the information it provides on our Universe and the chemical origins of life has an almost unique ability to engage the public and to inspire and enthuse the next generation to study science and technology. Therefore, in collaboration with partner organisations, such as EANA and Europlanet, members of the Action will bring some of the wonder and thrill of astrochemistry to the public.

B.4 Complementarity with other research programmes

Detailed investigation of astrochemistry demands the combination of laboratory and computational tools and close interaction with observational scientists. Expertise from astronomy, physical chemistry, spectroscopic and surface science must be assembled and coordinated for such a programme to develop. At national level, the benefits of such cooperation and collaboration have been recognised in France, Sweden, the Netherlands and the United Kingdom - where the AstroSurf Network funded by the Engineering and Physical Sciences Research Council, is an ideal illustrative example of how cooperation and collaboration may be assembled in a wider programme at a European level. Aspects of astrochemistry have formed part of European-funded programmes such as the Molecular Universe Training Network (dedicated only to gas phase reactions) and more recently it has been part of the ASTRONET observational network (combining resources of European telescope facilities) and the EuroPlanet consortia, which has reviewed the need for astrochemical data in the study of planetary atmospheres and sought to assemble a suitable on line database. EANA also has aspects of astrochemistry as part of its stated remit but at present its activities are limited to one annual meeting. As stated above, both EuroPlanet and EANA have indicated a willingness to collaborate with this Action in arranging joint meetings and workshops.

C. OBJECTIVES AND BENEFITS

C.1 Main/primary objectives

The main objective of this Action is to study chemical processes relevant to the physical conditions encountered in the interstellar medium, and on the surface and in the atmospheres of planetary bodies. The Action aims to provide new insights into the dynamics of the chemical reactions leading to molecular synthesis under such conditions and reveal how these are influenced by the ambient temperature and pressure.

Special attention will also be given to the study of the novel surface chemistry prevalent on interstellar medium dust grains and planetary surfaces. The Action also aims to combine such laboratory data with complementary chemical models to allow a fuller interpretation of observational data.

C.2 Secondary objectives

This COST Action will have considerable scientific and social impact by:

- Establishing a European forum to identify and characterise the challenges to be met and to assure Europe a leading role in the development of the rapidly growing area of astrochemistry.
- Bringing together the leading European groups with the different expertise needed to meet these challenges.
- Acting as a link between Europe’s academic research and space based research in this rapidly developing field.
- Acting as the necessary platform for young researchers to establish themselves in this field, thereby ensuring a continuity that will enable Europe to continue to hold a leading position in future development of this field.
- Coordinate and perform excellent multidisciplinary training for the next generation of space researchers.
- The organisation of a comprehensive compilation of available data for the European astrochemical community.

C.3 How will the objectives be achieved?

This Action will achieve its objectives by:

- Establishing coherent academic collaborations leading to development of pioneering research.
- Through exchanges of staff between participating groups.
- The development of interdisciplinary research projects.
- The establishment of a European coherent multidisciplinary training programme for students embarking on research in the field.

- The widening of the initial Action to form a viable research community by integration of other research partners and networks leading to the formation of a European Astrochemistry Network with European wide membership.
- The generation of further support from both national and international agencies.
- The dissemination of the work and objectives of the Action to wider scientific, political and public audiences.

C.4 Benefits of the Action

As stated in Section B, this Action aims to address what has been recognised as the major problem of incoherence in European research in astrochemistry by bringing together researchers from three different areas of chemistry (low temperature gas phase chemistry, heterogeneous chemistry and atmospheric chemistry). A COST Action provides the ideal forum within which researchers from these and related fields (e.g. surface science, aerosol/particulate research and chemical physics) can discuss the key scientific questions of modern astrochemistry and to develop an experimental framework within which these can be addressed. The workshops and annual meetings will be used to review status of the field and indicate suitable topics for collaborative research that may be developed through Short Term Scientific Missions (STSMs). The Action will also provide a valuable conduit for transfer of information on the facilities available in Europe including laboratories, computational models and simulations and data archives. Links to other identified ‘partners of choice’ will allow the astrochemistry community to interact with the planetary science community, space research and observational astronomy community. The Action will also play a crucial role in raising the profile of astrochemistry within both the astronomical and chemical research communities, and provide a modest, but much valued opportunity, for training and development of younger researchers by both workshops and scientific exchanges.

C.5 Target groups/end users

The major users of the results are expected to be the academic members of the astronomical, space science and planetary science research communities, over 100 of which have been contacted and indicated their interest in the Action. However, the Action has a wider aim of publicising the field of astrochemistry and identifying it as a new area of interdisciplinary research.

Therefore an important task of the Action is to disseminate its activities and describe the aims and objectives of astrochemistry to policy makers and the public. Dissemination is identified as an important role in the Action and will have a special consideration by the Management Committee. The Action aims to exploit 2009 as World Year of Astronomy to highlight astrochemistry's importance in modern astronomical research.

D. SCIENTIFIC PROGRAMME

D.1 Scientific focus

Recent space missions have highlighted the rich chemical complexity within the Universe. Over 160 molecular species have now been observed in the ISM within which stars and planetary systems are formed. Recent data have provided the first chemical maps of star and planet forming regions showing that chemistry is integral to such macroscopic structures. Similarly, within our solar system Europe's Huygens probe has provided a fascinating insight into the chemistry of Titan, the Saturn's moon whose atmosphere might be analogous to the one of early Earth, whilst intensive studies of Mars are revealing a rich chemical environment. The Action's scientific programme is aimed at exploring the chemistry prevalent under such conditions including:

1. Radical- and ion-induced reactions. At very low temperatures many room temperature reaction channels are inefficient and chemistry is often governed by so called barrierless reactions where the mechanisms are more akin to those encountered in collision physics - for example the formation of a complex between the reactants prior to the reaction product formation being similar to resonance formation in quantum scattering (e.g. the formation of transient negative ions in low energy electron scattering). Such reactions were probably the first chemical reactions to occur in the Universe, before the first stars were formed.

2. Heterogeneous chemistry. Although gas phase ion/radical chemistry may explain the formation of some of the small molecular compounds, it can not explain the formation of the most common molecule H_2 nor the larger organic compounds that are now being detected in the ISM. Such chemistry is now believed to occur on the surface of ice covered dust particles. Such chemistry is more akin to aerosol chemistry or modern nanotechnology than the traditional bulk surface chemistry and is likely to be strongly dependent on the morphology of the ice, about which we remain largely ignorant.

3. Planetary atmosphere chemistry. Once a planet has formed, much of its subsequent chemical evolution is determined by its atmospheric chemistry. The turbulence and physical processing of the surface by an atmosphere may lead to rapid change in the chemical nature of the surface and ultimately allow life to develop. Only now with our exploration of Mars, Titan and Venus, and their comparison with Earth, are we able to explore how chemical nature of the atmosphere may influence the subsequent evolution of the planet.

In more detail:

1. Radical- and ion-induced reactions. To date most laboratory chemistry has been performed under terrestrial conditions of standard temperature and pressure or under conditions pertaining to industry (e.g. high temperature combustion). In contrast, chemistry at low temperatures, e.g. the chemical reactions leading to ozone depletion in the stratosphere (200K < T < 270K) or the reaction dynamics at temperatures below 50K necessary to understand molecular formation processes in interstellar space, has only been investigated in the last few decades.

   Low-temperature chemical processes can usefully be divided into those with and without barriers. Reactions without barriers quickly become statistical and are conventionally described by capture theories. Reactions with barriers might be expected to become very slow at low temperatures, but in several cases substantial tunnelling rates persist even in the low-temperature limit. This is likely to be a general phenomenon, but requires full investigation. In particular, long-range potential wells exist in the entrance and exit channels of many reactions; such wells dramatically decrease tunnelling path lengths and increase tunnelling rates. Also, they create the conditions needed for scattering resonances and long-lived collision complexes. However, there are very few reactions for which the long-range wells are properly characterised and their effects understood. Developing our knowledge of the quantum nature of interactions/reactions is therefore essential to modelling such barrierless reactions and deriving rate constants which can be directly measured and tested in the laboratory.

This Action will encourage research that will lead to:

- The development of a better model of barrierless reaction dynamics (using quantum mechanical tunnelling) to predict reaction rates at low temperatures.
- The development of experiments with real molecular systems to measure low temperature reaction rates and compare with model simulations.

There are also many interesting phenomena involving low-temperature ions. Ion traps provide a different entrance to the ultracold regime, and low-temperature (5 -15K) ion-molecule reactions have been shown to be extremely important in astrochemistry, being one of the major mechanisms for molecular formation in the ISM. Ion-molecule reactions provide clear examples where long-range wells of physical forces are present before and after the barrier to reaction. These are typically handled by assuming that the dynamics over these wells is statistical. This assumption will fail at low energies and hence understanding such reactions is particularly important.

Cold molecular ion reaction processes can be investigated in ion/atom traps with the cold molecular ions produced either through interactions with a cold buffer gas or simultaneously trapping laser-cooled atomic ions and cold atoms/molecules. Cold ions may also be directly produced by photoionisation of atomic/molecular species in cold atom/molecule traps; indeed it is now possible to form ultracold plasmas within which such ultracold ion chemistry may occur. Furthermore experiments based on a single and highly spatially localised cold molecule are feasible and can serve as a unique target for laser assisted chemical processes.

This Action will develop:

- Experimental systems for exploring ultracold ion-atom and ion-molecule reactions.
- A theory necessary to interpret such results. For example, in the Wigner regime (and even at higher collision energies) the rapid acceleration due to ion-molecule polarization forces favours quantum reflection.

2. Heterogeneous chemistry. As evidence for the key role of heterogeneous chemistry in astrochemistry becomes increasingly apparent, several key questions have been highlighted:
   - To understand the formation of dust in the interstellar medium.
   - To understand the formation of simple molecules on model dust grain surfaces.
   - To understand the physical processes that result when an icy grain mantle is heated or irradiated with light, electrons or ions.
   - To understand the role of these processes on observations of grains, ices and the molecules formed by the intermediary of grains and their icy mantles in the evolving Universe.

New research topics in this area that may be developed by all Working Groups as part of this Action are:

Theme 1,formation of grains, small molecules and ices.

The topic of this research theme is to study the formation of dust grains and their optical properties, the formation of small molecules on grains, and the reactive accretion of icy layers and the morphological and spectroscopic properties of the resulting icy films. In particular to develop studies of:

- The mechanism of formation of interstellar dust grains from their initial condensation through to grain aggregate formation via grain-grain collisions.
- The release of reaction energy in the heterogeneous formation of small molecules on model dust grain surfaces leading to molecular products with high degree of internal (rotational/vibrational energy).
- The rates of ice formation on model dust grain surfaces.
- The morphology of ices formed on model dust grain surfaces.
- The infrared, optical and ultraviolet spectroscopy of ices formed on model dust grain surfaces.

Theme 2, physical processes in and on icy grains.

The primary aim in this theme is to develop a comprehensive understanding of the physical processes occurring when an icy mantle is subjected to electromagnetic radiation or bombarded with charged and/or neutral particles. Studies in this part of the scientific programme of the Action should focus on:

- Understanding the thermal desorption of both simple ices, complex mixed ices and clathrates as may be observed in the cold, dense regions of the ISM associated with star formation.
- Understanding desorption of both simples ices, complex mixed ices and clathrates induced through interaction with electromagnetic radiation from the IR to the soft X-ray.
- Understanding desorption of both simple ices, complex mixed ices and clathrates induced through interaction with low energy electrons and models of cosmic rays.
- Understanding the role of heat, electromagnetic radiation from the IR to the soft X-ray, and cosmic rays in promoting changes in morphology in icy films.

Theme 3, chemical tranformations in and on icy grains.

The topic of research theme 3 is to study the evolution and to simulate the formation of complex molecules of astrophysical interest on grains and in interstellar ices under laboratory controlled conditions with an unprecedented level of detail and sensitivity. This will require collaboration between astrochemists and surface scientists. The focus will be on:

- Ultraviolet (UV) photon- and low energy electron-induced chemical transformations.
- Vaccuum UV radiation, extreme UV radiation, and X-ray photon- and cosmic ray-induced chemical transformations.
- Chemical transformations following atom, radical or thermal molecular ion bombardment, using for instance special thermal cracking and microwave discharge sources.

Theme 4, modelling the gas-grain interaction.

Computational and simulation research should closely follow the empirical goals of themes 1 through 3 and focus on:

- Developing models for amorphous ices.
- Calculated IR and UV absorption spectra for water and adsorbates on and in crystalline and amorphous ices.
- Understanding the dynamics of photon-driven processes in amorphous ices, including photodesorption and photodissociation.
- Understanding molecular hydrogen formation on graphite and amorphous ice.
- Understanding the hydrogenation reactions of CO in various types of ice, particularly CH_3OH formation.
- Simulating diffusion of hydrogen atoms and oxygen atoms on hexagonal, cubic and amorphous ices.
- Simulating the condensation and growth of grains.
- Simulating the growth and evolution of water ice and other solids of relevant small molecules under interstellar conditions.

Theme 5, observations and astronomical models involving dust and ices.

The primary goal of this theme is to obtain quantitative astronomical constraints on the role of grains in interstellar chemistry. This requires a combination of observations and modelling. Research may include:

- Large and small scale maps of infrared lines of H_2 and deuterated species may be constructed to trace its formation on grain surfaces under different conditions.
- The assembly of an inventory of ices in different environments (temperature, density, UV) using infrared spectroscopy, e.g. the Spitzer Space Telescope.
- Search for the ultimate molecular complexity in space by radio, submillimetre and far-IR (Herschel) unbiased spectral surveys observations.
- A determination of the formation and lifecycle of water from gas to solid and back again by combining infrared spectroscopy of water ice with submillimeter spectroscopy of water gas from for example the Herschel Space Observatory.
- A study of the formation and composition of silicate and carbonaceous grains in disks and envelopes around young and old stars using infrared spectroscopy.

- Studies with high spatial resolution IR spectroscopy of photon-dominated regions in nebulae and around stars, looking at how the emission band strengths and relative intensities vary with distance from the exciting source as a diagnostic of polycyclic aromatic hydrocarbon formation and excitation mechanisms.
- Modelling of the gas-grain chemistry in hot cores and disks using the new laboratory data and compare with observations.

3. Planetary atmosphere chemistry. The study of planetary atmospheres is central to our understanding of astrochemistry, since it is inextricably linked to the goal of understanding where within the Universe those molecular systems that support the emergence of life are formed. The previous two themes (radical and ion-induced gas phase chemistry and heterogeneous chemistry) have concentrated upon molecular formation in the ISM, but the richest organic chemistry may in fact occur on planetary bodies and their moons. Such chemistry is different from that discussed before since both the pressure and temperature may be considerably higher and thus the chemistry is greatly altered. For example three-body collisions may play a role in the gas phase, leading in an oxygen rich atmosphere to the formation of ozone, itself a key molecule in sustaining life on a planetary surface. Aerosol chemistry may play a key role in regulating the physical nature of the planetary/lunar atmosphere and control the formation of clouds. It is only through unravelling the chemistry of planetary atmospheres that we may derive plausible biomarkers for life. These then can be used in exploration of exoplanets (planets around stars other than our own sun) in order to answer the greatest question of modern astrochemistry and astronomy - are we alone?

   The knowledge of the atmospheres of planets and lunar bodies in our own solar system has been greatly advanced by recent space missions (e.g. Mars Express and Cassini-Huygens to Saturn and Titan) providing a wealth of in-situ data that encourage the development of models of the planetary atmosphere and even their climate. However such models are often limited by lack of basic chemical data. The third theme of this Action is therefore to bring together planetary scientists, physical chemists and atmospheric modellers to develop improved models of planetary atmospheres in particular to:

   - Construct physical-chemical model of the Martian atmosphere and use this to predict its past climate

- Construct physical-chemical model of Titan’s atmosphere and unravel the composition and role of aerosols in is haze.
- To develop simulations of exoplanetary atmospheres with the aim of identifying characteristic spectral signatures that provide an indication of biotic processes.

Such a programme should exploit Europe’s growing capacity of planetary simulation chambers and computational infrastructure as supported by the EuroPlanet programme.

Finally, the problem of homochirality should be noted. Amino acids are the essential building blocks of all known life. They form the monomers from which all proteins, and thus all biological functions, are made. Perhaps their most striking feature is the curious fact that only the L-enantiomer of amino acids is used in the construction of proteins. It has been a matter of some debate whether this property of proteins is something that emerged during the evolution of life or if such molecular asymmetry is actually a prerequisite for life and stems from astrophysical or astrochemical processes. Since it has become increasingly clear in the last decades that there is a considerable variety of amino acids found in meteorites and that these amino acids, clearly of non-biological origin, show a dominance of the L-enantiomer, the debate seems to be more or less settled in favour of a non-biological process.

One model explaining the formation of amino acids and other organic chemical components is interstellar or circumstellar photochemistry on the surface of interstellar dust grains, but this model cannot easily explain the observed excess of one enantiomer of amino acids. There are two ways of inducing asymmetric photochemistry. One is asymmetric photo-synthesis in which a mixture of either racemic or non-chiral educts is transformed into chiral products with a chiral bias by means of circularly polarised radiation. The other way is asymmetric photolysis, in which a racemic mixture of chiral compounds is subjected to circularly polarised radiation which destroys more of one enantiomer than of the other.

Recent experiments have (i) explored the formation of amino acids in an ice mixture composed of H_2O, CO_2, CH_3OH and NH_3 under left-hand circularly polarised radiation, right-hand circularly polarised radiation and unpolarized UV radiation, and (ii) irradiated a racemic mixture of the amino acid leucin using UV radiation of different kinds of circular polarisation and wavelengths. These experiments show that decomposition in the photolysis experiment was very efficient. After 3 hours of irradiation, enantiomeric excesses of up to 2.6% were obtained. The experiment on asymmetric photosynthesis proved less conclusive, the enantiomeric excesses reached were in the order of magnitude of 1 percent. The effect was however the same whether right-hand circularly polarised light or left-hand circularly polarised light was used. A careful evaluation of the whole experimental procedures and analytical protocol showed that the margin of error in these kinds of experiments is also around 1%. Therefore it is not possible to determine if there is an asymmetric effect in the photo-synthesis.

D.2 Scientific work plan – methods and means

A COST Action does not directly fund the scientific research, but may play a crucial role in both coordinating and focusing a research programme such as that outlined above. As stated above, there is an urgent need for a forum within which the rapidly developing field of astrochemistry can be discussed and an interdisciplinary community assembled to pursue the necessary research agenda. In this Action the scientific work plan will be organised through a Scientific Programme Committee (SPC) in 3 Working Groups (WGs) (each dedicated to one of the three main themes discussed above and Section E). The Action will aim to review the current state of the art, for example by reviewing available data and thereby identifying deficiencies in the available databases (section H). Such reviews maybe organised through topical workshops hosted by the WGs, which will prepare reports and reviews for wider dissemination. The Action will place a major emphasis upon the support of STSMs, which will allow researchers to visit one another and conduct joint research projects. Past experience in other COST Actions has shown that a strong STSM programme leads to a strong scientific outcome in both publications and establishing longer term partnerships that produce a lasting legacy from the Action. The need for discussion and seed corn funding to establish such collaborations is particularly relevant for this Action, since astrochemistry research requires the assembly of research teams from diverse backgrounds who would be unlikely to meet in their normal research fora/conferences.

E. ORGANISATION

E.1 Coordination and organisation

This Action will provide an integrated research programme in the field of astrochemistry to incorporate both homogeneous and heterogeneous chemistry with atmospheric chemistry. The aim is to ensure that Europe is at the scientific forefront of a field that will form the focus of Europe's major space and planetary science research programme in the early 21st century.

To achieve this, a well organised, concerted Action is needed, which may only be achieved with an instrument such as COST that is dedicated to the coordination of the research and the promotion of the field. The organisational challenges of an ambitious interdisciplinary network are identified as the following:

(a) To enable and ensure effective communication between the members, particularly members from the different fields which synergy is essential for the success of this Action. This includes the dissemination of results as well as exchange on how to approach current issues and how to structure future research.

(b) To facilitate concerted collaborations between member groups with complimentary skills and capacities. Within the Action it is envisioned that such collaboration will be arranged through WGs, each dedicated to specific research topics (section D).

(c) To offer a forum to coordinate applications for research funds to national and European research foundations.

(d) To initiate collaborations between individual groups within the Action and to arrange training for younger scientists.

(e) To identify other European or international networks where information exchange or joint activities, such as workshops or training courses, are of value, and to initiate collaboration with these (for example ASTRONET, EuroPlanet and EANA).

(f) To motivate young researchers, involve them in decision making, and to encourage newcomers to join this exciting field.

(g) To organise training of students and young researchers in collaboration with other existing networks and organisations. This includes theme oriented workshops for young researchers.

(h) To ensure that the Action is flexible in the development of its scientific programme and open to new members, particularly new research groups developing in Central and Eastern Europe and those groups being established by younger academics.

The management of this project requires a clear structure to ensure all the aims are met. To achieve this, the Action will be organised through the Management Committee (MC) and a Scientific Programme Committee.

The MC will comprise up to two representatives from each of the participating member countries, and will include the Chair and the Vice-Chair. The MC will be responsible for the overall direction of the Action. The primary tasks of the MC are:

(1) Promoting the scientific activity of the programme.
(2) Enhancing the cooperation between members, stimulating/developing new joint studies and promoting the mobility of researchers (through STSMs).
(3) Providing opportunities for sharing instrumentation facilities and expertise between research teams for the pursuit of collaborative projects.
(4) Organising dedicated symposia and workshops to discuss current and plan future collaborative research, with an emphasis placed on oral presentations by younger researchers.
(5) Providing specialised training workshops concentrating upon cross disciplinary skills.
(6) Identifying other European and/or international networks where information exchange or joint activities are of value, and to initiate collaboration with those.
(7) Interacting with media and other organisations to promote the programme and to make it accessible to the general public and political decision makers acting on national and cross European levels.
(8) Arranging for training courses/workshops across the network and identifying and implementing best practice across the actions research fields to ensure that an adequate pool of trained researchers is incorporated into the research community at the end of the Action.
(9) Reporting and disseminating the results of the scientific research programme.
(10) Establishing and maintaining a functional web site for the Action (section F).

The MC will also be responsible for the administration of the Action's budget and preparing reports to the COST Office. The MC will also act as final arbitrator in the event of any disagreements amongst partners as to resource allocation, project tasks and dissemination of results.

The MC will be supported by the SPC, which will be responsible for overseeing the scientific programme including the establishment of the WGs, and the selection and review of the STSMs.

Many of the scientific themes are common to all the WGs and coordination and information exchange is essential for the success of the Action. Therefore an Annual Workshop will bring together all the major partners. For budgetary reasons one of the two MC meetings planned every year will be held at this Workshop. This annual meeting will be developed such that other international researchers may attend and present reviews of ongoing work. We also plan to have representatives from ESA. It is expected that the Annual Workshop will be arranged at venues close to and known to MC members. The Action should be willing to arrange joint conferences with other partners provided that the Action has a distinct entity within such conferences and can perform its necessary administrative, educational and PR functions.

E.2 Working Groups

The Action will be organised around three WGs:

i) WG1. Radical and ion molecule gas phase chemistry, which will explore ion molecule and neutral/neutral interactions at low temperatures both experimentally (using some unique laboratory facilities in Europe) and theoretically (developing quantum chemistry codes).

ii) WG2. Heterogeneous chemistry, which will be dedicated to investigating the chemical pathways within ice mimics typical of those in the ISM and on planetary surfaces processed by a range of external stimuli/radiation (UV light, electrons and ions).

iii) WG3. Planetary atmosphere chemistry. It will explore the chemistry occurring in planetary atmospheres through simulation of such atmospheres in laboratory facilities and within computational models.

Each WG will be open to members of the European research community who may apply to join. The primary purpose of the WGs is to provide a forum through which the Action can both strengthen and initiate contacts between the participating research groups. The WGs will host topical meetings on selected themes within their area to both review the current status of research in the field and propose new avenues of research. The WGs will also initiate/encourage staff exchanges for conduct of joint research projects.

On an annual basis the WGs will report to the MC (and SPC), which reviews the major scientific tasks of every WG and the overall tasks of the program. It is important for the success of this program to be able to react quickly upon the receipt of new knowledge and development of new technology. Therefore, the WGs may shift their emphasis during the life time of the Action.

Each WG will arrange annual meetings to prioritise monitor and review its own collaborative research programme. For budgetary reasons and to enhance interdisciplinary exchange, the WGs will be encouraged to have their annual meetings in conjunction with other WGs and dedicate time to coordination between the WGs. Furthermore, the WGs will be encouraged to offer special courses for young researchers in conjunction with their annual meetings and the Action will seek to offer partial financial support for these.

E.3 Liaison and interaction with other research programmes

These have been detailed in Section B. The Action will interact with EU Framework projects ASTRONET, a research infrastructure dedicated to observational astronomy (combining resources of European telescope facilities), and the EuroPlanet consortia which has reviewed the need for astrochemical data in the study of planetary atmospheres and sought to assemble a suitable on line database. Collaborations with EANA are also considered.

E.4 Gender balance and involvement of early-stage researchers

This COST Action will respect an appropriate gender balance in all its activities and the Management Committee will place this as a standard on all its MC agendas. The Action will also be committed to considerably involve early-stage researchers. This item will also be placed as a standard item on all MC agendas.

F. TIMETABLE

The total duration of the COST Action will be four years.

Table I: Timetable for the organisational bodies of the Action and the scientific meetings.

Legend; f; formation, m; meeting, mbf; meeting before the signified quarter, preferably in the preceding quarters signified by x, tws; training workshop.

	Year 1				Year 2				Year 3				Year 4			
1/4	1.	2.	3.	4.	1.	2.	3.	4.	1.	2.	3.	4.	1.	2.	3.	4.
MC	fm		m		m		m		m		m				m	m
SPC	f m		m				m				m					
WG 1	f	x	mbf/tws		x	x	mbf/tws		x	x	mbf/tws		x	x	mbf/tws	
WG 2	f	x	mbf/tws		x	x	mbf/tws		x	x	mbf/tws		x	x	mbf/tws	
WG 3	f	x	mbf/tws		x	x	mbf/tws		x	x	mbf/tws		x	x	mbf/tws	
Conf.			m				m				m				m	

Year 1 Initial meeting of the MC. Election of Chair and vice-Chair. First meeting of the SPC, which will organise the WGs. The WGs will all meet before the 3rd quarter of the same year to review the current state of the art and to define their tasks and the means to achieve them. In the third quarter of the first year, the first Annual Workshop will be held, at which the MC will meet to review the strategy to achieve the main goals of the Action. The SPC will review the annual progress reports of the WGs and to act upon them.

Year 2. The WGs will meet once and will host the first training workshops. The 2nd Annual Workshop will take place to which collaborative partners will be invited to present their vision of the benefits of the Action. The MC will meet in the 1st quarter and again at the Annual meeting in the third quarter. The SPC will also convene at the latter meeting. The STSM programme is expected to be most active in the 2nd and 3rd year.

Year 3. The third year will be organised similar to the second year. The WGs will meet at least once before the third quarter and will host training workshops. The themes of the training workshops for the third year will be identified by participating postgraduate and postdoctoral researchers during the second year and suggested to the MC. In the third quarter the 3rd Annual meeting will be held with strong representation of collaboration partners. The MC will meet in the 1st quarter and again at the 3rd Annual Workshop in the third quarter. The SPC will review the progress of the individual WGs and areas of overlapping work.

Year 4. The time table for the fourth year, which is the closing year of the Action, will be similar to the second and third year and will hold the Final Conference and MC meeting. It is anticipated that this meeting will take place at a major international conference that will be organised at the conclusion of the Action. This conference will be the pre-eminent conference on astrochemistry. A special volume summarising the Action’s research may be published as a Journal of Physics, Conference Series Volume.

G. ECONOMIC DIMENSION

The following COST countries have actively participated in the preparation of the Action or otherwise indicated their interest: AT, BE, CZ, DK, FI, FR, DE, GR, HU, IS, IT, NL, PL, PT, SK, ES, SE, CH and UK. On the basis of national estimates, the economic dimension of the activities to be carried out under the Action has been estimated at 80 Million € for the total duration of the Action. This estimate is valid under the assumption that all the countries mentioned above but no other countries will participate in the Action. Any departure from this will change the total cost accordingly.

H. DISSEMINATION PLAN

H.1 Who?

There are four main target groups for the dissemination of the objectives, the goals and the achievements of the Action:

- The participating researchers and the international science community.
- International organisations participating in the Action through collaboration with participating research groups (eg ESA).
- National and international policy makers and funding agencies for promotion of the Action.
- The general public to promote interest in the field and awareness of its potentials and at the same time to interest young people in science and to encourage them to choose that path as carrier.

Coordinated by the national representatives, the members will also contact their national policy makers and research agencies or representatives thereof, and will discuss possibilities of cooperation on the dissemination process. The national representatives will seek to identify and formulate ways to communicate the Action’s goals, means and objectives to those bodies and report them on the first MC meeting.

H.2 What?

All members will promote the Action on their research group’s home page and announce progress or achievements to the public media as appropriate. Such announcements will be made with reference to The Chemical Cosmos and the COST promoted international collaboration behind the Action.

The results obtained by the Action will be published in the refereed scientific literature. Computer programmes developed as part of the Action will be made available to Action partners and, where appropriate, also published. Data compilations will be published in book form. Interim reports and pre-prints of publications will be available electronically from the Action web page. The main purposes of the website are:

- To communicate news and announcements to the researchers participating in the Action.

- To allow rapid and effective reporting and dissemination of the results of the scientific research programme.
- To provide web based mailing-lists and archived discussion forum.
- Promotion of the project and to make it accessible to the general public and thereby to political decision makers acting on national and cross European levels.
- To create databases of articles, data and compile other information for knowledge transfer.

The web page will be partly password secured and allow upload of data, findings or interpretations for discussion. There will be a web based mailing list for members of the Action only, for discussions and rapid information exchange, and there will be a password protected databases of articles, data and other information for knowledge transfer. Activity reports, publications and news will be published on the non-protected part of the web page.

To accelerate decision making and for budgetary reasons MC, SPC or WG decisions may be taken at any time by electronic communication. The consensus on such decisions will be documented on the password protected part of the web page.

An annual scientific meeting will be held. This Annual Workshop will discuss scientific progress in all the strands and allow sufficient time for general discussion to enable new results to be reviewed and new research avenues to be debated. The majority of the talks will be given by the younger scientists involved in the Action and these who have benefited from Action hosted STSMs, which again will predominantly be younger researchers. The meeting will be open to all members of the Action with typically a few non-European researchers by invitation. At the conclusion of the Action, a major international conference will be organised (Final Conference). This conference will be the pre-eminent conference on European astrochemistry and will be open to non-network members. Conference proceedings may be published in collaboration with an international journal. A special volume summarising the Actions' research may be published in collaboration with Canopus books (a subsidiary of Springer-Verlag), which has recently commissioned a volume for COST Action P9 on Radiation Damage.

H.3 How?

Communiciations and web sites: Communications between members will be enhanced through a Newsletter. This will be circulated electronically and will include a quarterly report by each of the partners, abstracts of papers submitted for publication, meeting information and reports, adverts for postdoctoral positions, news of visits between nodes and a monthly review of latest international research papers in the electron induced chemistry (drawn from web of science database). An abbreviated version of the Newsletter will be available for to all international researchers upon registration. The Newsletter will be maintained on the Action's web site which will also include full details of the members, their research interests, ongoing research and personal profiles.

The Action will also collaborate with the astrochemistry.eu website, which has been developed as a forum to 'foster, broaden, and enhance the understanding of astrophysics and astrochemistry in its various forms like observations, laboratory and theoretical investigations'. In addition this site informs about conferences, symposia, seminars, other fora and special courses on the subject. General links to important databases or other sources of valuable information are given. This site is routinely cited by members of the international astochemsitry/astrophysics community. The COST Action will have a direct link to/from this site and provide a source of news stories (both informational and research). Building on this site we propose to use this site to establish an Annual Review of Astrochemistry.

Databases: The need for reliable comprehensive databases has been highlighted as being essential for the development of astrochemistry and the interpretation of much of the data now being collected by space and planetary missions. Requirements include: spectroscopic data for atoms, molecules and ions; chemical reaction rates (over a wide temperature range); cross sections including photoabsorption, photoionisation data, elastic and inelastic scattering cross sections for electron molecule interactions, and recombination cross sections for a large number of ions. However the assembly and support of such critical databases remains one of the major obstacles of modern astronomical research with many of the current astrochemical databases including sometimes outdated and often conflicting values.

Whilst several data bases are being developed (e.g. under the IDIS programme of the EuroPlanet network) and there have been two workshops this year devoted to critical evaluation of data on important astrochemical reactions, this COST Action will provide a forum for discussing how to assemble and regulate such databases in effect establishing an editorial board for such databases.

Summer University: An essential part of the Action is aimed at fostering a new generation of younger researchers with the interdisciplinary skills necessary for developing astrochemistry research, indeed this is vital for the longer-term sustainability of the field. Therefore the Action will seek to develop a European Summer University in astrochemistry to be held each year (e.g. in August) similar to that hosted by International Space University on the theme of space science. Topical summer schools and workshops are common to many networks involving typically 20-50 students, but we ultimately plan on a much wider scale. Rather than having a single course going through 1-2 weeks, we wish to host a multitude of different multidisciplinary courses relevant to astrochemistry, for example surface science, spectroscopy, planetary science, astrobiology and cosmology as well as technical topics on instrumentation, observational astronomy, data retrieval and storage, and computational models. Such a ‘summer university’ would be sufficiently large (100-200 students) that it would attract interest of the local general public such that it could organise public events in this summer university directed at a non-academic audience. The courses in the ‘summer university’ should be official courses and yield credits for the students under the new ECTS system. Being located in a different country every year, it will also attract students with other backgrounds and no previous involvement to the field. Such a ‘summer university’ requires long term planning and preparation and finances beyond those available in the Action, but much of the planning and discussion with other partners will be arranged under the auspices of the Action leading to further funding applications (e.g. in Framework programme) which may allow the first European Summer University in astrochemistry to be held in year 3 or 4 of the Action.

2009 World Year of Astronomy: 2009 has been designated World Year of Astronomy and the Action will utilise this opportunity to highlight to the general public and to policy makers alike that chemistry plays a critical role in astronomical research. This is not widely appreciated in contrast to astrophysics.

By developing a display explaining the chemical complexity of the Universe, the rich and diverse chemistry on planetary bodies and how chemistry is fundamental to the development and sustaining of life on any planet, the Action will seek to both publicise its aims and objectives and inform public, policy makers and young scientists (school and university students) of the need for research in this area while demonstrating the excitement and vitality of this still relatively new and underdeveloped field of study.