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

Brussels, 15 May 2014

COST 026/14

MEMORANDUM OF UNDERSTANDING

Subject :	Memorandum of Understanding for the implementation of a European Concerted Research Action designated as COST Action CM1401: Our Astro-Chemical History

Delegations will find attached the Memorandum of Understanding for COST Action CM1401 as approved by the COST Committee of Senior Officials (CSO) at its 190th meeting on 14 May 2014.

MEMORANDUM OF UNDERSTANDING
For the implementation of a European Concerted Research Action designated as

COST Action CM1401
OUR ASTRO-CHEMICAL HISTORY

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 4114/13 “COST Action Management” and document COST 4112/13 “Rules for Participation in and Implementation of COST Activities” , or in any new document amending or replacing them, the contents of which the Parties are fully aware of.

2. The main objective of the Action is to bring together astrophysical and chemical laboratories to focus on the molecular evolution towards complexity, from star formation to the present day Solar System, and to provide innovative experimental and theoretical chemical schemes.

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 48 million in 2014 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 section *2. Changes to a COST Action* in the document COST 4114/13.

A. ABSTRACT

A large variety of chemical compounds, from hydrides to complex organic species, is observed in star and planet forming regions. These complex species are also detected in present-day comets and meteorites, possibly as witnesses of the early stages of Solar System formation. An active chemistry proceeds in the harsh environments of pre-stellar cores and proto-planetary disks, where UV photons or X-rays irradiate cold diluted gases and ices, and radicals are copiously produced. The aim of this Action is to bring together laboratory and theoretical gas phase and surface chemistry as well as large facilities based experiments with the aim of rationalizing the molecular evolution. Specific markers, such as isotopic fractionation, ices composition, and abundance ratios of isomers, must be used and understood, in order to draw a coherent picture of our chemical origins. Succeeding former European initiatives that shaped the field of Astrochemistry, this Action focuses on the molecular evolution towards higher complexity. Being a stepping-stone for building models, the Action would deliver new schemes for physical chemistry at large, like chemistry of transient species and photochemistry, in gas or on surfaces.
Keywords: Astrochemistry, physical and quantum chemistry, gas phase chemistry, isotopic fractionation, surface chemistry and photochemistry, Solar System chemical evolution

B. BACKGROUND

B.1 General background

Chemistry is present in many harsh environments of our Universe. Molecules, and in particular organic molecules, have been observed in low temperature interstellar media, in star forming regions, in gases expelled by dying stars, and on the various types of grains that exist throughout our Galaxy. Also, in galaxies, local and in the early Universe, large reservoirs of molecules are observed. All these molecules were and are routinely observed mainly by the large infra-red, radio-telescopes and interferometric arrays.

Molecules are not only present in interstellar space, but they are everywhere present in our Solar System and in other planetary systems too. Many Complex Organic Molecules (COMs, defined here as molecules comprising at least on organic carbon atom - one CH bond- and one or several atoms of N, O, S), have been observed, like methyl-formate, acetamide, cyanopolyynes, a few cyclic organo-molecules. In our environment, they have been detected in comets, in meteorites, and evidently in the atmospheres of planets and satellites, by telescopes and space probes. However,

understanding in depth the ubiquitous molecular observations requires a complex combination of knowledge, stemming from astronomy, physics, and chemistry, the aim of this Action.
The space between the stars, the interstellar medium, contains very dilute gas and sub-micron sized dust grains, the material from which planetary systems form. In a first evolutionary phase, denser regions of this interstellar medium gravitationally collapse and form a protostellar core, surrounded by a flat rotating disk, the so-called protoplanetary disk. In a second evolutionary phase, coagulation processes within this disk lead to the formation of kilometre-sized bodies (planetesimals) and subsequent evolution eventually produces planets and smaller bodies such as asteroids and comets. During the first phase, the original interstellar material is heavily altered due to compression, heating, and intense irradiation with UV and X-rays. But also within the protoplanetary disk phase, significant processing occurs both in the gas phase as well as on the surfaces of dust grains.
In order to keep focussed, this Action deals with a specific, yet crucial problem: What is the fate of molecules between their synthesis in interstellar space and their subsequent detection in the present Solar System? What is our astrochemical heritage on earth? In a more specific way, the question arises: what is the relationship between these different stages of the evolution of matter, from the interstellar medium to Solar System-like environments? To what extent do organic molecules signal this evolution, and how do these molecules evolve in the very different environments they will encounter over time? Will they be kept frozen, will they react, and how complete are molecular inventories in star-forming environments that are progenitors of the Solar System of today? How do molecules cope with strong irradiation, with warming of the gases and evaporation of the ices during star formation, and with subsequent freezing in the comets?
Molecules serve as probes of the physical conditions in different environments, providing unconnected snapshots. This Action tries and links the gap between these different pictures by studying how simple molecules are formed, how they are destroyed under exposition to evolving extreme conditions, such as X and UV radiation and cosmic rays, and how they subsequently react either in gas phase or on the surfaces of ices to create new molecules of increasing complexity.
The European Union, some European Agencies (ESO, ESA, resp. European Southern Observatory and European Space Agency) and national or multi-national agencies, generously funded many ground based instruments and space borne probes and observatories, all aiming at exploring our "Molecular Universe", as the title of a preceding FP6 Research Training Network illustrated.
Europe has been for long and remains one of the major world actors in setting up experiments and observing astrophysical objects. Taking advantage of, and understanding the very numerous observations of these expensive instruments is an essential duty of the involved laboratories.

The story of the Complex Organic Molecules, synthesis, evolution, destruction, is the heart of this Action.

This Action aims at tackling the various problems of chemical evolution with methods of physical chemistry. Due to the unusual physical conditions prevailing in interstellar medium, new methods have to be developed in addition to existing ones. This is true for all areas of physical chemistry, in the laboratory, in chemical theory and also in modelling of the chemical networks kinetics. The areas identified as challenging are: (1) Low densities and temperatures ; (2) Interplay between surface and gas phase chemistry ; (3) Presence of high energy irradiation ; (4) Large variations of isotopic contents ; (5) Observables quantities of cations, anions, and open shell species. By treating these problems, *innovative physical chemistry will extend its domain of expertise* towards conditions rarely explored, experimentally and theoretically. These are for example: radical and radical ion chemistry in gas phase, radical and ion chemistry on surfaces, quantum effects, coexistence of very low temperatures and high energy irradiation.

Evidently, dealing with these question in a timely, relevant and quantitative manner requires bringing together of specialities existing in the various institutes of the COST Countries. In order to foster the community and to deal with the necessary involvement of the many chemical and astrophysical specialities, networking and community building are essential. While national initiatives exist, that fund research on various levels, previous networking initiatives proved extremely effective in solving old problems, and discovering new ones.

B.2 Current state of knowledge

COMs, were first discovered in the eighties in the warm (>100 K) and dense (density >10^6 cm^{-3}) gas surrounding high-mass protostars (hot cores) and with more recent instruments also around low-mass protostars (hot corinos). Several models were initially developed to explain the observed gas-phase abundances of COMs. The basic idea is that molecules such as H_2CO, CH_3OH and NH_3 form during the cold pre-collapse phase by the freeze-out of atoms or molecules on the grain surface (ice mantles) and subsequent hydrogenation through impinging H atoms. An important example is the hydrogenation of CO, which is predicted to lead to H_2CO and CH_3OH via successive additions of H atoms within the ice mantles. During the collapse, the forming protostar warms up the surrounding gas and dust leading to the partial evaporation of the ice mantles and returning some of these COMs into the gas phase.

The fate of the COMs synthesized during the hot core/corino phase is still debated. During the further evolution of the protostar, the hot core/corino envelope – the main reservoir of the COMs –

is dissipated, and formation of a flat rotating disk forms around the young star, the protoplanetary disk. In this disk, gas and ice mantles are further chemically processed through photochemistry, ion-molecule and neutral-neutral chemistry and at the same time coagulation of dust leads to the formation of larger km-sized bodies. Subsequently, gas giant planets and rocky planets form. Together with the rocky planets, a plethora of small bodies are formed, and populate the final planetary system. In the Solar System, theses are the asteroids and the comets, whose reservoirs are the Kuiper belt (beyond Neptune, at about 30 AU – Astronomical Units) and the Oort cloud (at about 10,000 AU).

The COMs formed during the hot core/corino phase can re-condense onto the ice mantles of grains in cold regions of the protoplanetary disk. Our understanding of large scale mixing and transport of matter in these disks is still poor. However, it is plausible to assume that part of that organic material will also participate in the formation of rocky planets and/or their atmospheres. Therefore, the hot core/corino chemistry can be highly relevant for our origins; it could influence and possibly even determine the chemical complexity that we observe today in our Solar System. The above observations show that organic chemistry in space must be extremely efficient and the main goal of this Action is to discover and quantify the main pathways behind it. COMs such as $HOCH_2CH_2OH$, $HCOOCH_3$, and NH2CHO are readily detected in comets through ground-based radio telescopes and space/planetary missions. Also, ions, both cationic and anionic, are detected in a wide variety of environments. More recently, the simplest amino acid, glycine, was detected by the STARDUST mission. The currently small list of COMs in comets will hugely increase with the new data from ROSETTA, the European cometary mission. In 2014, ROSETTA will reach the comet and start collecting data. The most pristine asteroids that reached the Earth, the carbonaceous meteorites, contain a variety of amino acids, some of which are not even naturally present on Earth. In the protoplanetary disk phase – intermediate between hot cores/corinos and comets/asteroids – observations of COMs do not yet exist. With ALMA (The Atacama Large Millimiter Array), that started partial operation in 2012 and will be fully operational in 2015, the detection of COMs in protoplanetary disks is likely around the corner.

Building on previous experience gained in particular in combustion and atmospheric chemistry, physical chemistry yielded essential information on the various COMs and their formation/destruction pathways. Both in theoretical and experimental work, several research themes were extremely fruitful: (1) Spectroscopy for identifying main species and their isotopomers; (2) Collisional coefficients, together with pressure broadening, to quantify excitation schemes; (3) Reaction rates, studied by molecular beam(s) for neutral reactions and ion/electron storage rings for charged species. Various levels of classical and quantum dynamics are able to deal with reactions involving open shell molecules, anions, cations and electrons. They have been used with some success, and are continuously developed. Surface chemistry is building on the tremendously important heterogeneous chemistry and catalysis needs. Most of these theoretical and experimental studies must substantially evolve in order to be able to tackle the problems of COMs in interstellar medium.

B.3 Reasons for the Action

This Action has three main complementary reasons, all based on the networking of active European research teams in chemistry and astrophysics: (1) It will develop and strengthen the common language, essential to understand the vast amount of data produced by existing or upcoming observatories, space probes and instruments; (2) It will link the critical manpower necessary for developing new physical chemistry methods ; (3) It will enhance the skills and networking of the present younger collaborators in the chemical physics laboratories, whether theoretical or experimental, helping them to be the next generation of researchers with a broad view point. They will deliver to the society at large the state of the art of the methods and data they discovered, bettered, and used.

This Action is absolutely timely: (1) The core observations for this Action relies on data coming from ground and space telescopes. For most large observational programs, data is private to the proposing consortium for a limited amount of time, less than two years usually. Having an established network of laboratories capable of using the data and exploiting it fully keeps the scientific content within the European laboratories. (2) The next generation of instruments and experiments are being designed/launched shortly, like the present ROSETTA cometary probe, the IR James Webb Space Telescope, and the new interferometer ALMA. In order to fully understand their flow of data and making effective consortia that affirm strongly the European presence, a fully established network of laboratory is a necessity. (3) The training of PhD students in physical chemistry within the language of these data is limited. This Action comes timely to decipher these data, provide models and educate now Early Stage Researchers.

The Action will also provide a central role in the organisation and dissemination of the chemical physics data generated during this Action, or else pre-existing but not widely known. Publications (preferably on the Action website) of proceedings of topical meetings (organised by the Working Groups) and the Annual Workshop will provide reviews of current research.

B.4 Complementarity with other research programmes

While many national agencies have special programmes to support either astrophysics / astrochemistry or evidently, physical chemistry, there are only few present programmes dedicated to the chemistry in the very peculiar environments. There is only one COST Trans-Domain Action (TD1308 “Origins and evolution of life on Earth and in the Universe (ORIGINS)), pertaining to exobiology. Cooperation and exchanges of ideas should happen between that Action and this one, in the form of shared invitations to meetings and possibly organising common Training Schools for Early Stage Researchers. While very different in nature, a few ERC projects deal with problems that are part of this network goal. Also, one FP7 ITN-People network used to be dedicated to laboratory astrophysics (LASSIE) and one COST Action (CM0805 “The Chemical Cosmos: Understanding Chemistry in Astronomical Environments”) dealt with small molecules. This Action builds on the experience gained thorough these networks, on the expertise and workforce of the ERCs. These large groups should be building blocks of this Action. Since the existence of this network depends on these national and international programmes, part of the research carried in those frameworks will be the backbone of this Action.

C. OBJECTIVES AND BENEFITS

C.1 Aim

The main objective of this Action is to bring together chemical and astrophysical laboratories to focus on the molecular evolution towards complexity, from the early stages of star formation to the present day Solar System. The Action will deliver knowledge and data essential to our understanding of the astrophysical data now being provided by the large European instruments, and provide innovative experimental and theoretical schemes for physical chemistry at large.

C.2 Objectives

Objectives within COST countries will be : (1) To establish and consolidate the community dealing with physical chemistry outside of the Earth, mainly during the formation of Solar type stars and planets around them; (2) To make the various ways of investigation (observation, chemical modelling, chemical experiments, chemical theory) share common goals, understand each other’s aims and objectives; (3) To allow Early Stage Researchers and researchers alike, to access intimate knowledge of chemistry and astrochemistry, all the more if one or the other is not their speciality, thanks to Training Schools, Short-Term Scientific Missions (STSMs); (4) To demonstrate to the various agencies specializing in funding astrophysics that chemistry is essential in understanding the ins and outs of the chemical and physical phenomena pertaining to star and planet formation, down to the present day comets and meteoritic materials; (5) To encourage young researchers to join this line of research, thereby ensuring both a continuity in the attractiveness of astrochemistry to prospective PhD students and post-docs, and also to attract post-docs from outside Europe to apply for positions, post-doctoral or permanent, in the various institutions of the COST Countries.

Outside of COST Countries, this Action will: (1) Demonstrate the ability of strongly bound communities to deal with complex problems, drawing on very different expertise, and scientific domains; (2) By making the COST Countries attractive to external students, post-docs, enforcing cooperation and exchanges, even helping in attracting new researchers.

C.3 How networking within the Action will yield the objectives?

As emphasized in parts B and D, this Action draws on many specialities inside and outside chemistry, on many particular laboratories, scattered all over the participating countries. Furthermore the approach is observational, experimental and theoretical. In order to get any meaningful result, to fulfil any of the objectives, very close networking is essential. Beyond the present point-to-point collaborations, a network allows for:

- Establishing long term multi-lateral collaborations on complex subjects needing several years of efforts.
- Enhancing the relevance of laboratory chemistry and theoretical chemistry for astronomy. It has been underlined by several prospective reports of the major agencies National Science Foundation (US), Astronet (EU), NASA (US), ESA Cosmic Vision (EU) underlined in their recent decadal prospective roadmaps, the absolute necessity of laboratory work to achieve major breakthroughs.
- The exchange of PhD students and postdoctoral fellow (by STSMs) will contribute to enrich their perspectives and establish future contacts.
- Organization of several Training schools, allowing Early Stage Researchers to get more in-depth knowledge and networking.
- By inviting colleagues/younger researchers from countries outside COST Countries, enhance the attractiveness of European research in general, and the themes of this Action in particular.

Previous experience, in particular through the past FP6 Research Training Network “Molecular

Universe”, the FP7 ”LASSIE”' ITN Network and the ended COST Action CM0805 “The Chemical Cosmos”, have very clearly shown the strong impact of networking. Thanks to those Networks and Actions, a new, strong community arose, that dealt with the astrophysical and astrochemical aspects of simple molecules in interstellar environments. These structures were -and still are- instrumental in defining the Key Observing for major European and international facilities. Today it seems impossible to take full advantage of the massive influx of data coming from multi-wavelength observation of astronomical objects, in the molecular spectroscopy, without having very different fields of expertise joined together, in a concerted way. The same is true for dissemination (see part H), since again, the work undertaken in the various laboratories takes its full impact by joint communications, papers, and proposals.

C.4 Potential impact of the Action

The aims of this Action are clearly of fundamental scientific nature, using instruments, which are at the tip of the current know-how, in astronomy, and physical chemistry. Hence, the main impact of the Action as a network of research laboratories is the increase of academic knowledge and innovation in physical chemistry in extreme environments. Cooperative work will certainly raise new questions about our own origins, to be tackled by younger colleagues in the course of their careers.

Research described in this Action is connected to observational facilities, funded by Europe and international agencies (space telescopes and probes, ALMA, ESO, IRAM –Institut de Radio-Astronomie Millimétrique). It is also dependant on very large instruments (like synchrotron radiation or free electron lasers, ion storage rings) and large computer centres. Accessing these instruments is limited. Also, improvements of these instruments, and their very design rely on large consortia of laboratories. An extremely important impact of this Action is the constitution of consortia, which would be capable of designing the future instruments for these facilities, and even propose future large instruments or space missions.

Methods and language developed within this Action are expected to be transferable to atmospheric chemistry, combustion chemistry, chemistry at solid-gas interfaces, and also FIR spectroscopy. Special care will be taken to have close interactions with those communities. Within some institutions, geophysical/geochemical laboratories have close relations with chemical or astrophysical ones. Such close ties are to be fully exploited.

Also, the evolution of molecules under exposition to energetic X and UV radiation and particles are of interest in medicine and biology to study the radiation damage, and the methods and data obtained in this work could be directly applicable. Reactions on ices and grains, even when focusing on small molecules are related to the field of nano-chemistry and again theoretical methods and experimental techniques developed in this Action are applicable.

C.5 Target groups/end users

The major users of the results are expected to be the academic members of the astrophysical and planetary science research communities. Of particular importance are the agencies that fund and supervise large instruments, telescopes and probes. The numerical databases and methods provided by this Action serve as a basis for judging proposals, defining experiments and instruments. These agencies are European or non-European, like NASA, JAPAN, ALMA, NRAO (National Radio-Astronomical observatory, NSF-USA). As a wider aim, this Action will provide data for chemical modellers of our Solar System, including the Earth. Learned societies are natural means for the end users to come into contact with the laboratories of this Action. Outreach activities are also planned to reach schools and the general public.

D. SCIENTIFIC PROGRAMME

D.1 Scientific focus

A. This Action builds on one specific core knowledge : *The observed spectroscopic presence in many astrophysical environments of Complex Organic Molecules* (COMs- molecules comprising organic carbon and at least one more heavy atom, C, N, O, S). More specifically, COMs are observed all along the evolution of stars, in the pre-stellar cores to the disk and jet environment of young stellar objects, in the protoplanetary disks as well as in the comets and Kuiper Belt Objects and some meteoritic materials, present in our present day Solar System. This core knowledge is a challenge for the chemical community, since synthesizing the observed COMs in the gaseous state or on the surface of grains has no one-sided explanation. Indeed, this Action focuses on the chemical processes at work at all stages, and on the way physical chemistry must be developed in order to take up the challenge presented by the mere observation of COMs, by their relative abundances and very peculiar isotopic fractionation. These problems are all the most difficult given that the astrochemical observations originate from media whose physical conditions are very far from those of chemical laboratories. Here are some of the challenges, which should be met by this Action.

1. Physical chemistry must be applied to gaseous and surface cold environments: COMs are observed at Tb 310 K. Are these COMs synthesized in situ on cold ice or are they the heirs of earlier chemistry, then vaporized by photo-desorption, or else synthesized locally when an external source of energy (photon, stellar wind or secondary electron, cosmic-ray) hits icy grains and dust particle? What are the plausible chemical pathways?
2. Astrochemistry is driven by kinetics, because of the gases extreme dilution (10^4 - 10^8 H atom cm^{-3}). However, reaction energetics (thermodynamics) are the final limitations, as cold surface or gas chemistry provide little kinetic energy, usually, less than a few tens or at the best hundreds of K. Also, because of the very low temperatures, tunnelling effects might play a decisive role.
3. Isotopic fractionation. D (^2H) and ^{15}N enrichments are well observed. D (deuterium) enrichment may be extreme and shows a huge variability, from 1 to 13 orders of magnitude, depending on the functionality, the molecule, and the physical media. Seemingly, ^{15}N enrichment varies with a facto of 1 to 10, depending on the nitrogen functionality. Theory and experiments have clues for these enrichments, but systematics are yet to be found.
4. Several types of star formation routes are observed today: oxygen-rich, anhydrous, carbon-rich. How to establish the carbon budget, and more generally, what are the evolution routes of molecules in the various star types? Conversely, to what extent do the abundances of some simple hydride molecules, like H_2O, NH_3, CH_4, influence the subsequent physical evolution (e.g., through their cooling properties) as well as the chemical evolution (e.g., by the abundances of reactive hydride radicals or cations/anions)?
5. Relative abundances of COMs, or, the great absentees. Some COMs present different isomers, like acetic acid or ethanol. It is not understood theoretically or experimentally why the most abundant isomers in interstellar media is often not the most stable, but rather another one, methyl formate or dimethyl ether. Is it due to some transition state or to the kinetics of formation, in gas or on the grains?
6. The role of UV and X-rays/cosmic rays is poorly understood, as they come as a supplementary variable complicating further more the points described above. A major question is the energy pathway, and how it affects both surface chemistry and possible outcomes, with emphasis on secondary electrons.

As this long list shows, these questions draw on various specialities of chemistry, experimental and theoretical. The laboratories joining the Action are experts in the techniques -in vitro and in silico- necessary to meet those challenges. They have their experimental/theoretical expertise, which is to be used for the peculiarities of COMs astrochemistry.

B. As importantly, the challenges to be raised in the Action go the other way around: ***The development of physical chemistry fostered by the challenges of Astrochemistry*** is an essential result by itself. As similar progresses were induced by very cold atomic and molecular physics (towards Bose-Einstein condensation) or, in a very different field, more in depth understanding of the chemistry of radicals pushed forward by chemistry in the upper terrestrial atmosphere, that led for example to a deep understanding of Halogen chemistry. In this Action, similarly, radical, radical ion, neutral chemistry is essential and not at all as thoroughly explored as closed-shell chemistry. Also, theoretical and experimental techniques adapted to reactions on very low temperature icy surfaces in vacuum could be seen in the light of heterogeneous chemistry and/or catalysis. Hence, a substantial enrichment of the physical chemistry toolbox is the second main goal of this Action, which is to put forward in WGs, meetings and dissemination expected in the course of the Action. Some of specific problems that are encountered.

1. Theoretically defining chemical pathways: what is the precision necessary for ab initio methods, are they reachable for realistic COMs problems? How to deal with tunnelling, is it possible to have rates in an approximate way?
2. Experimentally, is it possible/realistic to measure the rates of radical species reactivity and/or the branching ratios of reactions performed in beams?
3. How to extrapolate from experiments performed on the surface with the lowest realistic flux (atoms, photons) doable in the lab, to significantly lower fluxes expected in the astrophysical environments. Which sensitivity are the experiments to reach?
4. Theoretical methods that predict the surface chemistry of atoms like H or O as well as the reactivity of heavier species, and in particular their hydrogenation (or deuteration)?
5. Coupling the surface and gas chemistry, with the huge difference in absolute abundances, while still having manageable (and economical) modelling and plausible model outcomes.

It must be underlined, though, that the models *do not aim at high precision,* in general: The observational astrochemistry yields orders of magnitude, factor of 2-3 are the norm, even in relative numbers. Hence, all the theories, experiments, and models, which aim at reproducing and understanding these numbers, must keep in focus the inherent poor precision of astrophysical understandings.

D.2 Scientific work plan methods and means

The Action is built on four WGs, each specific of a particular chemical process. The four WGs are outlined below; some specific problems to be treated for each of the stellar evolution stages are also indicated.

(1) *The theoretical methods* to be used depend strongly on the size of the system and the nature of the process to be studied, whether studying only the ground, or excited electronic states. For small systems and few electronic states, high level *ab initio* methods will be used to generate a potential energy surface, necessary for the full understanding of the reaction/excitation Exact quantum methods, either time-independent close coupling or wave packets (as Multi-Configurational Time Dependent Hartree method) will be used to obtain the rates for collisions and photodissociation processes. Larger systems require the use of classical trajectory calculations and when quantum effects are important, such as tunnelling or zero-point energy, semiclassical methods or analogues will be used, such as molecular dynamics path integral like methods.

As the system grows bigger, this approach becomes impractical. First, Density Functional Theory (DFT) methods is one possibility to treat icy particles. Other possibilities remain open. The reaction dynamics when using DFT on large systems could possibly be on the fly, calculation DFT points all along the classical dynamics. This can be used to get rates, and may also provide ideas to construct reduced dimensionality models to perform quantum dynamical simulations. The highest level of complexity arises when considering photochemical reaction on ices, since it involve many atoms and very excited states.

(2) *The experimental methods*

The main challenge from an experimental point of view is to reproduce interstellar conditions: the average kinetic energy is typically confined to 0.8 kJ mol^{-1} (corresponding to a temperature of 100 K) in diffuse clouds and 0.08 kJ mol-1 (corresponding to a temperature of 10 K) in dark molecular clouds. In other words, the formation routes of molecular species can only involve processes without appreciable activation energy. Furthermore, the number density is so small that only bimolecular collisions can occur. Needless to say, it is very difficult to reproduce the chemistry under the conditions of the interstellar medium in laboratory experiments.

As far as neutral-neutral gas-phase reactions are concerned, essentially two experimental approaches have been used, which reproduce either the low energy or the low density environments. In particular, the CRESU (the French acronym for Cinétique de Réaction en Écoulement Supersonique Uniforme) technique, which makes use of supersonic expansion to cool down the reactants mixture, has made it possible to measure the rate coefficients of bimolecular

processes involving either ions or one/two radicals down to very low temperatures (as low as 10 K). Nevertheless, the CRESU environment is not collision free. The best experimental approach to simulate low density environments relies on the Crossed Molecular Beam (CMB) technique, which allows to characterize the reactive collisions under collision free conditions. With this method, secondary and wall conditions are completely avoided. While it is difficult to derive integral cross sections and rate coefficients from CMB experiments, the information provided by this technique on the nature of the primary reaction products and their branching ratios is invaluable.
Ion molecule reactions are also extremely important in the chemistry of Inter-Stellar Media (ISM), because they are usually characterized by very large rate coefficients. The employed experimental techniques are in most aspects similar to those illustrated for neutral-neutral reactions. One important experimental approach regards the study of electron-ion recombination because most of the observed species are indeed neutrals and, were ion molecule reactions the main synthetic routes of complex molecules, a final step that converts the ions into neutrals is necessary. Ion–electron recombination reactions are much more difficult to study in the laboratory than are ion–molecule reactions, especially when it comes to establish the dissociative products. In those experiments it was established that electron-ion recombination often leads to extensive fragmentation of the ion.
Heterogeneous reactions such as those occurring in the icy mantles of dust grains are especially challenging, but have been carried out in different labs with great success. Formation pathways of many interstellar molecules on grain surface have been identified, although in many cases it is still too early to decide for many key molecules if they are formed in the gas phase or via surface processes.
The exchange of methodologies, problems and solutions among the communities of ion-molecule, neutral-neutral and surface chemistry research groups will lead to experimental innovative solutions. For instance, the merging of the expertise in the production of radicals and ions can pave the way to the study of ion-radical reactions, a class of reaction very poorly characterized in the laboratory. The COST Action will be of great help in promoting the collaboration between experimental and theoretical groups.
The Action is built on 4 WGs. These WG are chosen by dividing the whole evolution in processes. Each of the 4 identified processes occur in all the physical stages of matter and COMs evolution. The goal being to provide a unified view of the whole evolution, each of the WG must interact strongly with the others. However, each of the WG retains its own specificity and technicality.

WG1 Chemistry in cold diluted gas

Cold gas phase chemistry pertains to all astrophysical environments targeted in this COST Action.

The pre-stellar phase is characterized by gas and dust in dark (only cosmic ray irradiation) cold (10-30 K) and low density (10^3-10^5 cm^{-3}) conditions. The same type of conditions are found in dark cold parts of hot cores/corinos and the outer cold regions of protoplanetary disks (beyond ~100 AU).
In cold gas, the usual laboratory experiments are not meaningful. Specially designed experiments and theories are set up and their results incorporated in the large gas-phase chemical networks, such as UMIST University of Manchester Institute of Science and Technology) or KIDA (Kinetic Data for Astrochemistry). This WG of the Action will specially take care of ion and radical reactions, theoretically and experimentally. Also, collision excitation rate for COMs, necessary for quantitative analysis of abundances, are within the WG1 scope.

WG2: Icy grain surface chemistry

An important and sometimes debated role is given to the surface of grains. The grains are covered with ices, sometimes dubbed 'dirty water ices', because of the many impurities. WG2 aims at studying the chemical reactions on grains, in the cold regions of the ISM. Also of interest are the conditions and reactions that occur when the ices sublimate, in more evolved stages of stellar evolution. Many experimental set-ups try and study these mechanisms, focussing often on ad-atom chemistry and build up of larger molecules and COMs. An important aspect of the WG will be the relevance and reproducibility of the laboratory surface chemistry, and the possible reliable theoretical approaches.

WG3: UV and X-ray photochemistry

WG3 focuses on modelling and measuring the rate constants for photo-dissociation and photoionization by UV and X-ray photons and cosmic radiation. The group will also study light induced processes on the surface of dust grains. The focus will be both theoretical and experimental. The WG will favour molecules that can be detected in space, especially in comets, and will emphasize the understanding of the reaction mechanisms.

WG4: Isotopic fractionation

In comets, inter planetary materials and carbonaceous chondrites meteorites, as well as star forming regions in various evolutionary stages (from pre-stellar cores to protostars to protoplanetary disks), molecular species have been found enriched in the heavy isotopes deuterium (D) and nitrogen-15 with deuterium enrichments wildly varying, from 1 to 13 orders of magnitude. There is also a general tendency for organic molecules to display larger D-fractions compared to water, while ^{15}N-fractionation is more active in nitrile- than amine-bearing molecules. Recent results from the

Herschel Space Observatory have shown that the HDO/H_2O abundance ratio in comets is essentially the same as that in our oceans (about ten times larger than the D/H cosmic ratio). The observational tools (spectroscopy, collisional rates) and theoretical tools are to be developed to understand existing observations, forthcoming ones and actual experimental data.

E. ORGANISATION

E.1 Coordination and organisation

To achieve its ambitious goals, this Action has to rely on a well-balanced coordination and management. In order to do so, the Management Committee (MC) and the Scientific Program Committee (SPC) will be set up. The SPC comprises members of the Action whose advice will be sought at least at mid-term and at general meetings, and in any case of necessity, for particularly demanding scientific questions.

The MC is responsible for

1) Promoting the scientific activity of the Action, by means of: (a) Enhancing the cooperation between members; (b) Actively promoting the use of STSMs amongst all kinds of researchers: advanced, mid-career and early-stage researchers (ESRs); (c) Putting together resources, codes, experimental techniques which enhance the overall productivity.
2) Organising meeting: (a) General scientific kick-off, mid-term and final general meetings, with well-balanced Scientific Organising Committees; (b) Annual specialized meetings of each WG
3) Providing specialised Training Schools, workshops, especially targeting ESRs.
4) Ensuring the permanence of the information produced in the meetings, by means of electronic information and publication. Making sure that COST is acknowledged in publications resulting from collaborative work carried out within the Action and in outreach activities.
5) Promoting the set-up and maintenance of a website, whose content reflects the activity of the Action.
6) Interacting with media.
7) Interacting with other networks, European or International in order to promote the visibility of the Action.
8) Whenever possible encouraging the presence of Action members at national or international meetings of relevance, including Learned Societies.
9) Maintaining close contacts with non-European specialised networks/learned societies sections, whose goal is to promote astrochemistry and physical chemistry, as envisioned in this Action.

The MC is responsible for the management of the Action’s budget and will prepare the reports to be submitted to the COST office. The MC is responsible for overseeing the day-to-day scientific activity, including the functioning of the WGs, the material and scientific organisation of the meetings as well as the selection and review of STSMs. For budgetary reasons, the annual MC meeting will be coinciding with the General Meeting, whenever possible. All the meetings will be arranged sufficiently in advance to reduce travel costs and to places suitable for such meetings with a balance given to all participating countries/laboratories. During MC meetings update on the budget status and progress report of the WGs will be presented. A member of the MC, will be designated as responsible for outreach activities; another MC member will be responsible for the training schools, their publicity and the websites of those schools.

E.2 Working Groups

Four WGs constitute the backbone of this Action. They cover together the actual history of matter from pre-stellar cores towards present-day Solar System (see section D, for their detailed scientific contents). The WGs are organised by chemical themes, so that all aspects of the peculiar chemistry in cold and rarefied environments are duly dealt with.
WG1: Chemistry in cold and diluted gas. WG: Icy surface chemistry WG3: UV/X photochemistry
WG4: Isotopic fractionation
All WGs will be targeting close cooperation between chemistry and astrochemistry. Their scientific management, their meetings will be balanced between the 3 pillars of this Action –chemistry, modelling, observational data. Each WG is open to participation from any researcher of the participating COST Countries, who may apply to join one or several WGs.
Topical meeting, with participation of 2 or more WGs, will be programmed, especially in the second half of the Action, if the necessity arises. The topics of the WG meetings, and of the sessions in the general meetings will be decided by the MC, the WG Leaders, and with relevant advices of the SPC. They will nominate, if necessary, a special SOC (Scientific Organising Committee) who will take care of inviting the speakers of the meeting, taking special care at balancing the invited speakers between the various sub-specialities.
The Action will organize training schools, preferably in the first half of the Action, so that ESRs get a better benefit from the ensuing collaborative work.

E.3 Liaison and interaction with other research programmes

As underlined on part B4, few present European networks deal specifically with the goals of this

Action. The main exception is the COST Action TD1308 “Origins and evolution of life on Earth and in the Universe (ORIGINS). Cooperation with this Action is envisioned, for example a joint training school could be organised.

The Action will also establish contact with relevant European agencies or transnational initiatives (ESA, ESO, and IRAM).

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 item 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.

The Action involves prominent female researchers at all levels, and at various stages of their career. They will represent role models, motivation and encouragement for female young researchers in natural sciences. The Action will take special care in inviting female researchers and early-career researchers to contribute to Action activities.

F. TIMETABLE

	Year 1		**Year 2**		**Year 3**		**Year 4**	
	1st sem.	2nd sem.	1st sem.	2nd sem.	1st sem.	2nd sem.	1st sem.	2nd sem.
Whole Action	Kick off	Training school 1			Mid-term		Training school 2	Final
WG1		Meeting	Meeting			Meeting		Meeting
WG2		Meeting	Meeting			Meeting		Meeting
WG3		Meeting	Meeting			Meeting		Meeting
WG4		Meeting	Meeting			Meeting		Meeting
MC	Meeting		Meeting		Meeting			Meeting
SPC	Meeting		Meeting		Meeting			Meeting
Outreach event		Event			Event			Event

Year 1. The scientific Kick-off meeting will take place as early as possible, to launch the Action,

make a series of state-of-the art talks, present to ESRs the on-going work. WG will be launched. A training school on general aspects of chemistry in astrophysical conditions will be organized.
Year 2. WG meetings with emphasis on the chemistry-astrophysics interface, will be held separately or jointly. WG2 and WG3 will have a joint meeting, on surface chemistry and photochemistry.
Year 3. Mid-term general meeting: first results, detailed contacts with end users: databases, external organizations.
Year 4. Training school, with emphasis on astrochemistry and databases proper use. Final general meeting.

G. ECONOMIC DIMENSION

The following COST countries have actively participated in the preparation of the Action or otherwise indicated their interest: AT, CZ, DE, ES, FR, HU, IT, NL, PL, SE, SK, UK. On the basis of national estimates, the economic dimension of the activities to be carried out under the Action has been estimated at 48 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?

1. This Action is extremely interdisciplinary in nature. This implies that several scientific communities will benefit from this Action: experimental and theoretical chemists, astronomers, astrophysics, physicist, and statisticians.
2. The Chemical Community at large is concerned by the new pathways that would be opened by scientists working in this Action.
3. The topic of this Action is of interest to national and international (e.g. ESA, ESO) agencies and observatories. They will interact with the Action and therefore will be the beneficiaries as well as the promoters of our dissemination plan.
4. Younger students are tomorrow scientists and tomorrow general public. It is of great importance for this Action to target students, both High School and junior University students.

5. The general public will be one of our major target of the Action. Members of this Action have experience with in outreach activities with the public in general, through conferences, media interactions, and website production.

H.2 What?

For scientists, the material to be disseminated is of three categories: scientific work, suited for professional publication in peer-reviewed journals or conferences, numerical data pertaining to physical chemistry, and codes, suitable for modelling. For Students, the dissemination aims mainly at: making the work carried out within the Action (astrochemistry, physical chemistry) attractive for younger students (from the age of 14 approximately), in order for them to appreciate how science is progressing in a new and exciting field. For the general public, description of the results, as well as breakthroughs must be publicized; the astrophysics community has a long history of websites and newsletters managing; this Action will build on that experience.

H.3 How?

The dissemination of the Action deliverables will depend on the target audience. Using the three types outlined in the previous section, we shall adopt the following means.
To the scientific community: the members of the Action belong to institutions whose dissemination policy is very strong with in house press offices, as well as Outreach departments, Institutional websites, and Departmental ones. The data to be opened up is:

- New scientific work. The usual professional publication of new results, in peer-reviewed papers is the essential dissemination tool. It has proved extremely effective and long-lasting; in the past, astrochemical results published in major journals are always highly cited and have a very long citing life. Making those publications valuable for large communities. Also, actively participating in conferences, with junior and senior scientists presenting their work, is a well-known way to allow other communities understand astrochemical ways of thinking. Also, publishing in main journals and participating in large conferences make the topic of this Action highly visible to prospective students and colleagues alike.
- Training Schools organised during the course of this Action should have their materials put online, on the website of the Action.

- Actual data. One of the aims of this Action is to produce numerical data, to be incorporated in models, existing or internally developed. The data (rates, thermodynamics and energies of chemical pathways) is to be incorporated in large data bases, like LAMDA and Basecol, the chemical networks (UMIST, KIDA), the modelling codes (PDR codes, general chemical codes).
- Codes. Numerical codes developed during the course of the Action will be published and made available through the usual pathways: website, publications.

There will be a dedicated website which will be used to advertise and promote the COST Action, with relevant links to the official COST website. Members of the Action will link the Action website to the one of their institution in order to display News on the COST Action ‘Our Astro-Chemical History’. Annual meeting will be organised to discuss the scientific progresses in all sub-disciplines covered by the Action. Enough time will be allocated to presentations given by the younger members of the Action and for parallel discussion sessions.

Following the frequency of the meetings, a newsletter dedicated to this COST Action will be produced: this will be in electronic form only and will contain (i) a report on recent(s) COST meetings, a list of funded STSMs, and (iii) post-doctoral and job adverts in the several fields of research involved in this Action.

To National and International Agencies and Societies: The members of the Action will actively make frequent contact with their individual national agencies and as well as astronomy and chemical societies promoting the COST Action, informing them about relevant scientific results and more importantly making use of their press offices.

To the general public: The ‘Our Astro-Chemical History’ Action will be well represented in public events that take place in many countries and institutions. The Action will actively encourage each member of this Action to participate in radio and TV interviews as well as contribute to dissemination via blogs. Also, there is some experience within the Action for producing 'YouTube videos' and other Social Network posting.