Toward a Dutch Astrochemistry Network

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Preamble

This working document is written in preparation for the NWO astrochemistry meeting on October 7th, 2009. The goal of this meeting is to organize the Dutch astrochemistry community and this document provides a framework for the discussion that day. Eventually, this document may evolve into a full-fledge proposal to NWO. For now, the science program has been identified into which the Dutch astrochemical expertise and interest can be naturally be divided but that may well be adjusted at the meeting. Table 1 provides a preliminary attempt to summarize this Dutch expertise in astrochemistry. As for the science program, this summary will be served well by a critical evaluation at the meeting.

1. Background

The origin and evolution of the molecular universe starts with the injection of material – much of it in molecular form – by stars in the later stages of their life, the subsequent processing of this material in the interstellar medium by the prevalent ultraviolet radiation fields, energetic particles, and strong shocks, and ends with the incorporation of this material into newly formed stars and their budding planetary systems. In this way, the chemical processes taking place in the interstellar medium may eventually be inherited by planetary systems. During this evolution, molecules exert a direct influence on their environment. Molecules dominate the cooling of gas inside dense molecular clouds. Molecules also control the ionization balance in such environments and thereby the coupling of magnetic fields to the gas. Through their influence on the forces supporting clouds against gravity, molecules also affect the process of star formation. Large molecules are also thought to be a major contributor to the heating of diffuse atomic gas in the interstellar medium and thereby the physical conditions in such environments and the phase structure of the interstellar medium.

Hence, molecules are directly interwoven into the fabric of the universe. They are an important component of the Universe and play a central role in many key processes that dominate the structure and evolution of galaxies. Understanding the origin and evolution of interstellar and circumstellar molecules is therefore a fundamental goal of modern astrophysics.

Over the next five years, European ground-based and space-based missions will open up the universe to high spatial and spectral resolution studies at infrared and submillimeter wavelengths. May 2009, the European Space Agency has launched the Herschel Space Observatory with the heterodyne instrument, HIFI, – developed by an
international consortium under PI-ship of the Dutch space agency, SRON – that will open up the THz frequency regime for systematic studies of the molecular inventory of space. The European Southern Observatory, ESO, is a major partner in the construction of the sub-millimeter interferometer, ALMA, in Chili. This interferometer will provide unprecedented spatial resolution at sub-millimeter wavelengths. These new observatories will allow us to study, in much greater detail, the composition and the origin and evolution of molecules in space. Moreover, molecular transitions in these spectral ranges provide a sensitive probe of the dynamics and the physical and chemical conditions in a wide range of objects at scales ranging from budding planetary systems to galactic and extragalactic sizes. Hence, these missions provide us with the tools to study key astrophysical and astrochemical processes involved in the formation and evolution of planets, stars, and galaxies.

Over the last few years, new physical chemistry methods have been developed that carry the promise of opening up new avenues of research in astrochemistry. These include, for example, a double-resonance hole-burning spectroscopy scheme developed at the FOM institute in Nieuwegein for the study of bioactive molecules that can be adapted for infrared absorption spectroscopy of large molecular species of astrophysical relevance. At the Sackler Laboratory in Leiden, UHV surface science set ups have been build to study the key chemical processes that control surface chemistry in the formation of interstellar ices under cryogenic conditions. At the Laser Center of the Vrije Universiteit, an optical cavity ring-down plasma experiment has been put together that mimics interstellar clouds for optical spectroscopy of hydrocarbon radicals in relation to the Diffuse Interstellar Band problem. On the theoretical side, Moore’s law enables ever larger systems to be accurately treated. In particular, Density Functional Theory techniques have steadily improved and allow now accurate calculations on the IR vibrational spectra of large (100+ C-atom) molecules. It is also now possible to model solid state processes using molecular dynamics techniques on systems containing some 500 molecules. These developments in chemical physics and molecular physics allow us to address now questions and systems that were not possible even only 10 years ago.

Analysis and interpretation of the data that these new missions will make available in terms of the physical and chemical characteristics of the astronomical sources will require detailed astronomical modeling tools supported by laboratory measurements and theoretical studies of chemical reactions and collisional excitation rates on species of astrophysical relevance. Progress in this area will require close collaboration of scientists active in molecular physics, astronomy, and chemistry. The Netherlands has been an active player in the field of astrochemistry for many years. However, the many Dutch astronomy, molecular physics, and chemistry groups active in this area, largely contribute from their own perspective. Here, we propose a highly multi-interdisciplinary network combining the astronomical and chemical expertise in the Netherlands with the goal of understanding the origin and evolution of molecules in space and their role in the Universe. This goal will be reached through a highly integrated and coherent program of astrochemical and astrophysical experiments, quantum chemical calculations, and laboratory spectroscopy of astronomically relevant species in combination with an active program on modeling and observations of astronomical sources.
2. Science Program

Building upon the knowledge, expertise and experience of astronomy, molecular physics, and chemistry groups active in the field of astrochemistry in the Netherlands, we propose four major science themes. In this section, we will summarize these themes and their objectives. These themes give rise to a detailed workplan that will be developed in a bottoms up approach starting with a kick off meeting on October 7, 2009, and that will be described in section 3.

2.1 The Aromatic Universe

Over the last decade, the presence of large molecules in space has been well established through their infrared emission signatures (eg., the IR emission features) and their visual absorption bands (eg., the Diffuse Interstellar Bands). Their charge state is a balance between photo-ionization and electron recombination. Photons also play a fundamental role in determining their overall lifetime through photo-dissociation of the carbon skeleton and the production of specific fragments. The other process that is thought to play a key role in the evolution of large molecules is the interaction with energetic particles in shocks. Through their effect on the energy and ionization balance of the gas, these large species play an important role in the diffuse interstellar medium of galaxies, photodissociation regions created by massive stars interacting with their environment, and in protoplanetary disk surface layers.

The focus in this research area will be on combining laboratory and quantum chemical studies with astronomical observations and models of interstellar sources to explore the evolution and the physical and chemical characteristics of large molecules in space, including in regions of star and planet formation. This includes studies on the importance of UV photolysis and shocks for the chemical evolution of large molecules. In addition, this study will be supplemented by laboratory and quantum-chemical spectroscopy studies on astronomically relevant species. The emphasis in this effort will be on large PAH molecules and carbon chains.

Key objectives include:

- What are the key (photo)chemical reactions of large PAHs and carbon chains in the interstellar medium?
- What is the relation between the chemical and physical characteristics of large molecules (structure, size, charge state, excitation) and the physical and chemical conditions of a region?
- What are the spectroscopic signatures of large molecules in space?
- What is the role of chemical processing involving large molecules in the physical evolution of the Universe?
2.2 The Reactive Universe

The interstellar medium is a harsh environment for molecules, differing in many respects from traditional terrestrial and laboratory settings. The extreme conditions of space – specifically the low density and temperatures, the long timescales, the strong UV field, and the energetic particles – give rise to a unique chemistry resulting in a highly unusual organic inventory with – beside simple hydrides and oxides – a diversity of unsaturated species, radicals and ions. Chemical routes in the interstellar medium involve photodissociation, as well as ion-molecule or neutral-neutral radical reactions, such as dissociative recombination, collisional dissociation, ion–molecule exchange, and charge-transfer reactions. These interstellar species are observed through their electronic transitions – generally in absorption – in the visible and ultraviolet or through their pure rotational transitions – commonly in emission – in the (sub)millimeter range. Excitation of these transitions occurs mainly through collisions with the thermal gas atoms predominantly H, H₂, and He but fluorescence by nearby stars can also populate higher levels. Studies of these species provide direct insight in the chemistry in space. In addition, the myriad of transitions each with their own excitation characteristics provide unique insight in the physical conditions of the emission/absorption zones and make molecules a unparalleled probe of the Universe.

The focus in this research area will be on combining laboratory and quantum chemical studies with astronomical observations and models of interstellar sources to understand the chemistry of radicals and ions in space. In addition, experimental and theoretical studies on the excitation will be undertaken to develop molecular observations as a tool for studies of the Universe. The emphasis in this effort will be on simple radicals and ions and a link with the previous topic is the study of aromatic cations and anions.

Key objectives include:

- What are the roles of radicals and ions in the chemistry of the interstellar medium?
- What is the excitation of such species in space and what can observations tell us about the physical and chemical conditions of a region?
- How do such species affect their environment?

2.3 The Icy Universe

Inside dense molecular cloud cores, most of the gas phase species (except for H₂ and He) accrete onto dust grains, forming a thin ice mantle. These species can react among themselves on the grain surface, converting for example oxygen into water and carbon monoxide into formaldehyde and methanol. UV photolysis as well as cosmic ray bombardment can further process these ices. Polymerization reactions driven by thermal processing due to nearby newly formed stars provide another channel towards molecular complexity. In this way, simple gas phase species are transformed into a complex chemical mixture. Besides removing much of the molecular cooling agents
from the gas, interstellar ices are also thought to greatly facilitate the coagulation process of sub-micron-sized interstellar dust grains – the first step towards planet formation. Similar chemical processes may also play a role in the cold, outer regions of protoplanetary disks – the birthsites of cometary bodies. In the Solar system, icy cometary bodies may have played a vital role in delivering the volatile inventory to the terrestrial planets.

The focus in this research area will be on combining laboratory and astrochemical studies with astronomical models of interstellar sources to explore the evolution and the physical and chemical characteristics of interstellar ices in regions of star and planet formation with the emphasis on UV photolysis, atom/ion bombardment, and thermal processing of astrophysically relevant ices. In addition, this study will be supplemented by laboratory spectroscopy studies on astronomically relevant species. To this end, experiments will be performed to understand the elementary physical and chemical processes involved in the origin and evolution of interstellar ices and this understanding will be translated to the astronomical reality through detailed models and will be tested by astronomical observations.

Key objectives include:

- What are the key chemical routes on interstellar grain surfaces?
- What is the role of energetic processing of interstellar ices in driving molecular complexity?
- What are the spectroscopic signatures of interstellar ices?
- What is the role of chemical processing involving interstellar ices in the physical evolution of regions of star and planet formation?
- What is the role of PAHs and radicals in the solid state?

2.4 The Prebiotic Universe

Life on Earth is generally thought to have started with a period of prebiotic chemistry in which the molecular building blocks of life were formed that could then be self-assembled into replicating systems. Part of this prebiotic chemistry may have taken place elsewhere and delivered to the early Earth by accreting planetesimals or cometesimals. Indeed, carbonaceous chondrites show a diverse organic inventory betraying a rich chemistry on the parent body from which these meteorites were derived. Likewise, the warm and dense gas associated with regions of star and planet formation are replete with relative simple organic species such ethanol, dimethylether, methylformate and glycolaldehyde that may be signatures of interstellar prebiotic chemistry. Besides reactions in the warm gas, this may involve chemistry on grain surfaces and the formation of interstellar ices and subsequently modified by gas phase reactions when the newly formed star sublimes these ices. Astrochemistry provides the link that connects prebiotic chemistry with astronomy and understanding the role of *interstellar chemistry* in the drive towards molecular complexity and the start of prebiotic chemistry is a key goal.
Key objectives include:

- What are the key chemical routes towards molecular complexity in regions of star and planet formation?
- What is the organic inventory of regions of star and planet formation particularly in the habitable zone?
- What does the organic inventory of regions of star and planet formation tell us about the chemical history of Solar system objects such as comets, meteorites, and interplanetary dust particles?
- How can we differentiate between interstellar prebiotic chemistry and the molecular “signatures of life”?

3. Work Program

Detailed workplan. To be developed by the Dutch astrochemistry (in the broadest sense) community starting on the kick off meeting October 7, 2009.

4. The Network

4.1 Research disciplines

The field of molecular astrophysics is a highly interdisciplinary field where molecular physics, laboratory spectroscopy, surface chemistry, theoretical chemistry, astrochemistry, astronomical observations, and astronomical modeling intersect. Each of these science areas is characterized by the use of different techniques and methods and no single individual scientist or even single institute covers all these areas to the depth required. Table 1 summarizes relevant expertise of the different institutes in molecular astrophysics in the Netherlands. This table is an indication and is not meant to be complete. In the past, collaborations involving members of these teams have successfully addressed key questions within molecular astrophysics. However, the next step will have to come from a wide ranging, coherent, and integrated program on the basic physical and chemical processes driving astrochemistry. This program will have to bring together experts and institutes from all of these scientific disciplines. In that way, Dutch science can be expected to reap the full benefit of the new developments in the field of chemical physics and molecular physics and prepare adequately for the exciting, new, observational opportunities on the horizon. Because relevant expertise is spread over so many different institutes, coordination is best done at the national level through an integrated Dutch Astrochemistry Network. Indeed, the objectives and work program that form the core of the scientific goals of the network fully demonstrate the inherent interwoven nature of this field of research. In this way, the very distinguished Dutch record in the area of molecular astrophysics – evident, for example, at international conferences – can be extended into the next decade.
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4.2 Organization

The research in the network has been divided into four global science themes. Each of these topics will be covered “end-to-end”; e.g., will cover the topic from astronomical data and modeling to molecular experiment, modeling and data. Hence, each of these themes is a joint task and, for successful completion, requires contribution from the physics, chemistry, and astronomy groups in this network. These contributions have been split out as specific milestones and the main team and leader responsible for that milestone have been identified. Thus, several teams contribute their specific expertise and experience to a science theme and these teams will have to collaborate for a successful completion of their task.

Work on specific milestones will be supported through the appointment of graduate students and/or postdocs. We envision that the research by these graduate students and postdocs will be highly interdisciplinary. Specifically, we expect that each PhD student in chemistry will be involved in the astronomical side as well and will have at least one “astronomical” chapter in his thesis and vice versa. Publications will be in

![Organization Tree Diagram](image-url)
astronomical and chemical physics/molecular physics/spectroscopy journals. These appointments may be shared between several teams if that facilitates work on the milestone(s). The appointments will be made at the home institute of the team leader and this team leader will be responsible for the supervision of the work of the appointed fellow. A second supervisor will be appointed to cover the other expertise the student is involved in. The local institute where the fellow is appointed will manage the financial aspects of each appointment.

Each science theme has a coordinator who will be responsible for coordinating the activities in this area. Interaction between the different science themes will be the responsibility of the coordinator.

The network may coordinate and integrate its activities with international groups active in molecular astrophysics. This can be at the level of specific milestones and may include exchange of team members and/or students and postdocs. It may also involve organization of joint meetings. The network coordinator will be responsible for the coordination of these international activities.

The four science theme coordinators together with the network coordinator form the executive committee of the network. The executive committee is responsible for the overall operations of the network and will decide on the allocation of resources within the network. The overall functioning of the network and progress towards the goals and objectives of the network as well as the overall allocation of funds within the network will be yearly reviewed by an international board of outside experts in the field of molecular astrophysics. The advice from the board will be made available to NWO.

### 4.3 Network and Communication

The science of this network is highly interdisciplinary between the fields of physics, astronomy, and chemistry. The key to success for this network will therefore reside in a high degree of collaboration between the individual teams at the working level to ensure cross-fertilization between the disciplines. Indeed, the strength of the network will reside in the way it will be able to create informal and formal interactions and exchange of information and ideas between the different science disciplines involved in astrochemistry. Communication within the network will be facilitated through a Twiki page for informal discussions as well as a “living space” for working documents. In this environment, all members of the network will be able to deposit and modify documents. The website will provide access to progress reports, intermediate results, and the final results of the research involving this network. The network will also maintain a website open to the community in which they will report their progress and that will also serve as outreach to the general public.

Each of the four science topics will organize at least yearly a meeting at the national level where progress on its milestones will be discussed. The network will organize an annual workshop where the overall progress of the network will be presented to and reviewed the advisory board. In addition, this annual meeting will be used to bring in external experts to brief the teams on new developments in the science disciplines involved in astrochemistry. At the end of the contract, the network will
organize an international conference at which it will present its results to the larger community. Some funding will be set aside at the coordinator’s level to support attendance of foreign experts at these meetings. However, the home institutes will managed travel funding for the appointed fellows and the team members.

The network will organize a summerschool each year – taught by team members and outside experts – to train the appointed graduate students and postdocs in all of the techniques and methods relevant to molecular astrophysics.

The network will actively promote participation of international visitors through small travel grants.