Molecular astrophysics

A volume honouring Alexander Dalgarno

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A VOLUME HONOURING
ALEXANDER DALGARNO

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Frontmatter
More information

CONTENTS

Part VI H_2 in regions of massive star formation

Part VII Molecules near stars and in stellar ejecta

Part VIII Moderately ionized gas and chemistry at large redshifts

DEDICATION

Until about 20 years ago, almost all of our knowledge of astronomical sources derived from observations of the emission and absorption of radiation by neutral and ionized atomic species and by electrons moving in the fields of such species and in large-scale magnetic fields. A large fraction of the astrophysics done up to that time could be described as atomic astrophysics. Of course, nuclear astrophysics was another important area of inquiry, but much of that field's database came from observations of stellar spectra formed by atomic processes.

In 1967 when Alex Dalgarno moved to Cambridge, Massachusetts and began to devote a substantial fraction of his efforts to theoretical molecular astrophysics, CH, CH^+, and CN, which had been observed close to 30 years earlier in optical absorption against stars, and OH, which had been seen recently in emission at 18 cm, were the only molecules to have been detected in the interstellar gas. It was anticipated that H_2 would be observed in ultraviolet absorption against nearby massive O and B stars, and Alex began calculations to investigate quantitatively molecular processes important in the destruction and pumping of molecular hydrogen by the interstellar radiation field. This work made possible the construction of models of diffuse interstellar molecular clouds. Thus began a long term effort to develop molecular astrophysics into a rigorous field of investigation.

Molecules exist in a wide variety of astronomical sources including interstellar clouds, star-forming regions, ionized nebulae, stellar atmospheres, the pregalactic medium, quasar absorption line regions, very young supernova remnants, and the interstellar media and the centers of other galaxies, including many with active nuclei. Though the subjects of this volume are restricted to more distant objects, molecules also exist in extraterrestrial sources, such as planetary atmospheres and comets, in the Solar System. Alex has led efforts to understand the chemistries which form the molecules in this wide variety of sources, to use their abundances

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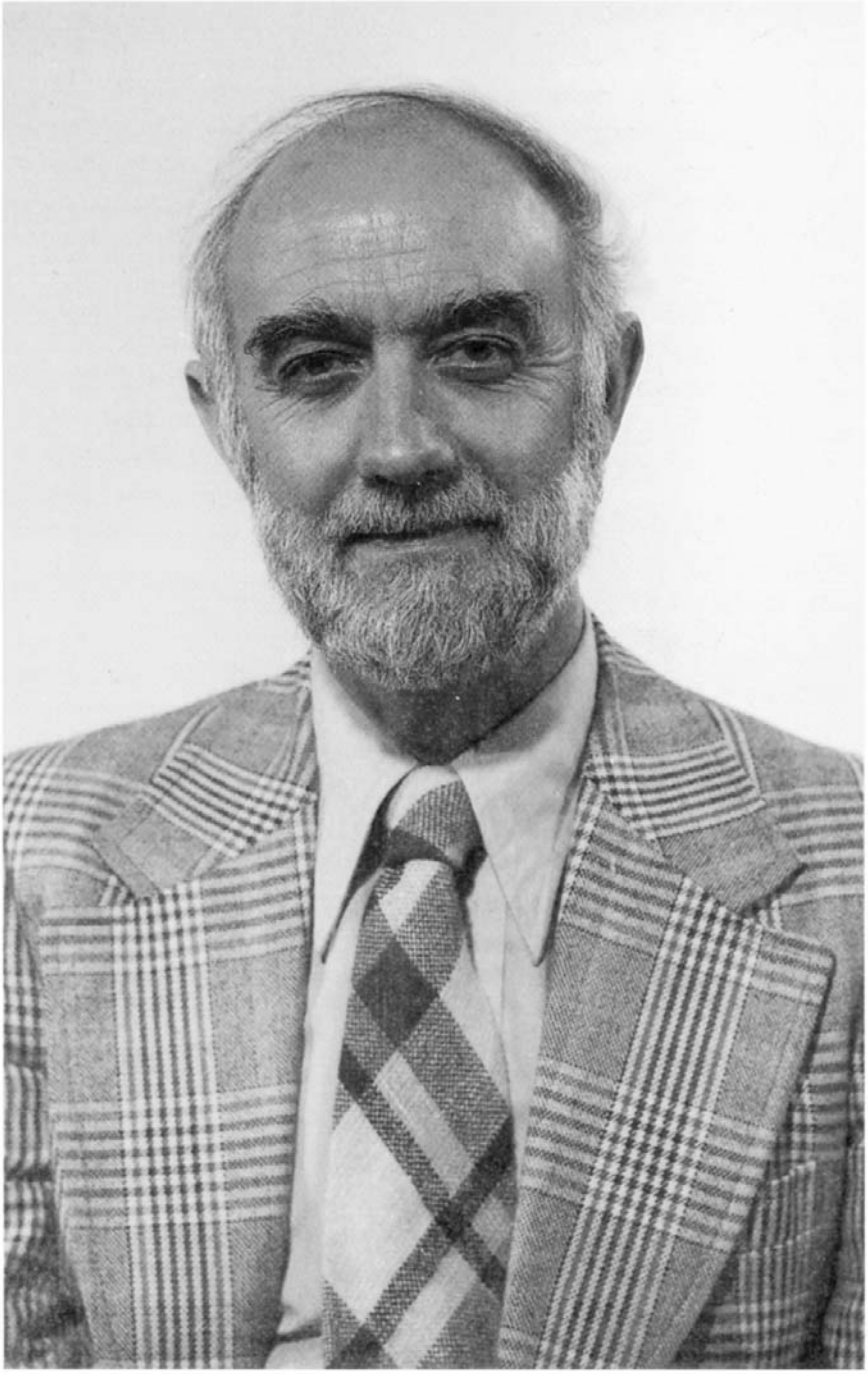

and level populations to diagnose the macroscopic properties of the sources, and to elucidate the roles which they play in regulating those macroscopic properties.

In 1986, he was awarded the Royal Astronomical Society's Gold Medal for his success in these efforts.

Over roughly 20 years, Alex has created and maintained an important school within theoretical astrophysics. Most major active contributors in theoretical molecular astrophysics have been Alex's students or collaborators or have been influenced significantly by working together with one or more of his former students and close associates. Most of Alex's work in theoretical astrophysics has been concerned directly with understanding or using data, and he has interacted with a number of leading observational molecular astronomers as well.

Alex had already led a distinguished career as a theoretical atomic and molecular physicist and as an atmospheric physicist before moving to the States. He has continued to publish prodigiously in those areas and received the Hodgkins Medal of the Smithsonian Institution in 1977 and the Davisson–Germer Award of the American Physical Society in 1980 for his work in them. Indeed, Alex is highly regarded in the four separate communities of physicists, astronomers, chemists, and atmospheric scientists. Alex has profitably used his background in these other areas when conducting his astrophysical investigations. His knowledge of atomic and molecular processes and ability to study them quantitatively, his experience and facility in identifying the dominant physical and chemical mechanisms in complicated plasmas, and his skill in suggesting to laboratory physicists and chemists astrophysically relevant measurements have contributed to his impact as a molecular astrophysicist.

Students constitute a group which has benefitted from Alex's attention. In the mid-1970s, when I studied with him and he was the chairman of the Harvard Department of Astronomy, Alex possessed the reputation of being able to match a project with the constraints of a student's abilities and the available time and of being a faculty member to whom a student facing difficulties could turn for help. He seems to make availability to students a special priority. Despite his own supply of problems, Alex always has been extremely encouraging to his students when they have pursued projects of their own devising. He is an excellent teacher capable of getting students started and supporting their growth as independent research scientists. His help even extends to the teaching of English composition, a useful but sometimes harrowing experience for the instructee.

Alex's personal qualities suit him for more than his role as mentor. They make him a valued companion as well. His humour is dry and playfully interactive and sometimes seems to serve as an affectionate means of communication with friends. Alex combines quiet modesty with a confidence which can reassure others. His words to those of his students and friends who confide in him during moments of real or imagined crisis are sympathetic and wise.

He is an excellent sportsman. The possibility of becoming a professional soccer player existed before he suffered an injury. He is known to be one of the best squash players in astrophysics, and he plays tennis at least as well as any of his former students. When its existence was threatened by a building project, the Observatory tennis court was mentioned to the Harvard-Radcliffe executives as having been one of the benefits which had attracted him to Harvard; happily, the Observatory personnel still have access to a tennis court, and the construction led to the existence of squash courts a short walk from Alex's office.

A book on the subject of molecular astrophysics would be improved by a contribution by Alex. However, one of the two purposes (the other being to provide a self-contained introductory overview of the field which he has played such a dominant role in shaping) of this collection is to honor Alex who on 5 January 1988 celebrated the sixtieth anniversary of his birth in London. In addition, the 1988 volume of *Advances in Atomic and Molecular Physics* consists of papers dedicated to Alex and the January 1988 issue of *Planetary and Space Science* contains contributions written in his honor. These two works should also be consulted to obtain a more complete overview of his scientific influence and other biographical information.

The importance of Alex's research was also recognized when he was elected a Fellow of the American Academy of Arts and Sciences in 1969 and a Fellow of the Royal Society in 1972. He obtained his higher education in University College, London, where he took his Ph.D. in 1951 and from 1951 through 1966 held faculty posts in The Queen's University of Belfast where he was promoted to a chair in 1961. Both of these institutions have honored him; the former by electing him a Honorary Fellow in 1976 and the latter by awarding him an honorary D.Sc. in 1980.

Currently, Alex is a physicist in the Smithsonian Astrophysical Observatory and the Phillips Professor of Astronomy in Harvard University. He is the editor of *The Astrophysical Journal Letters*.

As alluded to above, Alex's theoretical work reflects the approach of an empiricist. In recent years, he has advocated efforts to ensure the future of theoretical atomic and molecular physics in the foremost physics research departments in American universities. He believes 'that physics is embodied not in its equations, but in the solutions to the equations.'

PREFACE

The present volume has been designed to be a self-contained introduction to the field of molecular astrophysics. It can serve as the text for a one semester postgraduate course concerning that subject exclusively or as a supplementary text in a postgraduate course on the interstellar medium. It can also be used by research astronomers, atomic and molecular physicists, chemists, and atmospheric scientists who have interests in weakly ionized plasmas and the physical and chemical processes which occur in them and who wish to become familiar with recent work in molecular astrophysics.

Many of the articles concern theoretical studies and modelling. Part I, consisting of two chapters written by observers, provides a general description of the astronomical context within which much of the remainder of the volume should be considered. The contribution by Per Friberg and Åke Hjalmarson reviews briefly our understanding of the global physical properties of the Galactic interstellar medium, describes the wide range of conditions within the dark molecular clouds (those having visual extinctions greater than about 1) and the distribution in the Galaxy of the dark clouds, and compares the chemical contents of different regions in various dark clouds. Leo Blitz has written about observations of molecules in other galaxies including some with active nuclei.

The study of chemistry in diffuse molecular clouds (those having a visual extinction of about 1 or less) constitutes the subject of Part II and is perhaps the most fundamental area in molecular astrophysics. Before beginning Part II, the reader who is unfamiliar with the structure of and spectra of diatomic molecules may wish to turn first to the article by Kate Kirby in which an introduction to those topics is given. Many of the data for the diffuse clouds have been obtained in absorption studies against background stars.

Direct measurements of the H_2 rotational level population distributions and of the H column densities are used to infer the detailed physical properties in diffuse molecular clouds. The H_2 is formed on the surfaces of grains and is destroyed by a photodissociation process involving excitation of higher electronic states which radiatively decay to the rovibrational continuum of the ground electronic state. Radiative decays of the higher electronic states to the discrete rovibrational levels of the ground electronic state also occur and the subsequent radiative cascades through the rovibrational ladder are generally assumed to be responsible for the production of the H_2 detected in the $v = 0, J = 3$–6 levels. The populations of the lower levels are determined by collisional processes. Diffuse cloud modelling is the most rigorously based theoretical enterprise in molecular astrophysics and is reviewed in the paper by Ewine van Dishoeck who also has described efforts to construct low temperature equilibrium models of the diffuse cloud chemistry to account for the measured column densities of a number of simple diatomic species. The chemistry in diffuse clouds is often initiated by the photoionization of atomic species. Because oxygen has an ionization potential exceeding that of atomic hydrogen, there are no ultraviolet photons which can ionize O (implying on diffuse clouds); rather the oxygen chemistry is driven by cosmic ray induced ionization, but once O^+ is formed it reacts quickly with H_2 and eventually OH, the abundance of which is used to infer cosmic ray ionization rates, is formed.

CH^+ and CO are two species which have measured column densities which are much higher than those explained easily with low temperature equilibrium models. In roughly the past fifteen years, the interstellar medium has come to be viewed as a site of violent activity, as mentioned by Per Friberg and Åke Hjalmarson. Consequently, the effects of shocks on diffuse cloud chemistry have been considered. Bill Langer has reviewed critically the observations which give insight into the dynamics and structures of diffuse clouds and, hence, constrain shock models. David Flower, Guillaume Pineau des Forêts, and I have summarized work on the chemistry in diffuse cloud shocks. Because high temperatures ($T \gtrsim 10^3$ K) and ion–neutral streaming can drive reactions which are slow in cold diffuse clouds, shocks have been considered as the sites of formation of molecules including CH^+. Multifluid hydromagnetic models are appropriate for shocks in weakly ionized clouds. The chemistry affects the ionization and shock structures. Because H_2 is collisionally excited in shocks, the observed H_2 level populations constrain models. Neither current low temperature chemical equilibrium models, existing shock models, nor a combination of them seem compatible with the H_2, CH^+, and CO diffuse cloud data.

Part III concerns the chemistry of dense clouds. Tom Millar has written an introduction to the area in which he has described the basic gas phase chemical networks including the processes which determine the ionization structure and chemical fractionation. Cosmic rays are the sole source in dense clouds of the ionization which drives the chemistry. His paper and the one by Ewine van Dishoeck should provide the reader with sufficient background to appreciate the importance of many of the studies described in Part IV. He also has summarized results of steady state and simple time dependent models of dense cloud chemistry. Dust is also a component of molecular clouds and contains a substantial fraction of the heavy elements in them. Chemistry occurs on dust grains as Victoria Buch has discussed. One of several important ways in which dust grains can affect the gas phase chemistry is by removing electrons. Stephen Lepp's article concerns, in part, the effect of small grains or large molecules on the gas phase ionization structures in dense and diffuse clouds. His contribution could have been included in either Part III or Part II. It also contains a discussion of diffuse cloud heating due to photoabsorption by grains. In Part IV, the paper by Evelyne Roueff addresses some of the collisional processes which give rise to radiative losses which balance the heat input into clouds.

Part IV contains contributions dealing with the molecular processes which must be included in models and which produce the spectral features which originate in the molecular clouds. Kate Kirby has provided a short introduction to the structure of diatomic molecules and their spectra and has discussed the mechanisms by which photoionization and photodissociation of molecules occur. As noted above, absorption data provide much of the information known about diffuse molecular clouds and photoionization and photodissociation are processes which are extremely important in establishing the ionization structure and molecular abundances in those clouds. David Smith, Nigel Adams, and Eldon Ferguson have reviewed the experimental techniques used to obtain data relevant to diffuse cloud and dense cloud modelling and have discussed results for several classes of reactions and their relevance to chemical modelling. Sir David Bates has summarized our theoretical understanding of various types of reactions. The modelling of diffuse and dense cloud chemistries relies very heavily on experimental and theoretical studies of the chemical processes. Evelyne Roueff has described theoretical studies of collisional excitation processes. Rotational excitation of molecules results in the radio and millimeter emissions which have been observed to study molecular clouds. A detailed knowledge of collisional excitation mechanisms is often necessary for the diagnosis of cloud conditions. The internal level population distributions in reactants in the laboratory differ from those in reactants in molecular clouds, and Margaret Graff has considered the ways in which the level population distributions affect some astronomically important reactions.

Parts I–IV acquaint the reader with the basic fundamentals of molecular astrophysics and some of the classic, often unsolved, problems. The subsequent parts deal primarily with special topics and particularly challenging outstanding questions.

The theme of Part V is the presence of atomic species in dense clouds. In his review of the observations of neutral and singly ionized atomic species in dark clouds, Gary Melnick has pointed out that while some of the emission from such species is associated with regions in which ultraviolet radiation from stars dissociates molecules and ionizes atoms, some of the emission is extended. He has noted further that a number of viable explanations have been suggested for the means of producing neutral atomic carbon, the emission of which has been studied with sufficient resolution to gain some idea of its spatial extent in M17 and ρ Oph. One of those suggested explanations is that dissociating stellar radiation is able to penetrate deeply into clouds either because they are clumpy or because the far ultraviolet dust opacity is lower than usually assumed. Wayne Roberge has described the detailed radiative transfer theory necessary for the construction of models in which the photodissociation of CO is responsible for the production of the observed neutral carbon. His paper describes a general formalism which is of importance for diffuse cloud modelling and for the modelling of dense H_2 photodissociation zones as discussed by Amiel Sternberg in Part VI. An additional source of photodissociation and photoionization in dense cloud has been considered by Roland Gredel and arises because ultraviolet photons are emitted following the collisionally induced excitation of H_2 by energetic electrons produced by cosmic ray induced ionization. He has summarized the effects of this process on dark cloud chemistry and has calculated the expected neutral atomic carbon to carbon monoxide abundance ratio. Note that Tom Millar has included a briefer discussion of the same process in his article in Part III. Another class of explanations for the neutral atomic carbon in 'apparently quiescent' regions is based on the assumption that the regions are, in fact, dynamic. Steve Charnley and David Williams have written about the chemistry in a region, which if it were further away would appear quiescent but in which the gas is thought to pass repeatedly through a dynamical cycle. The chemistry in that region, Barnard 5, probably does not attain equilibrium and the dynamical processing may ensure that atomic carbon is abundant. Barnard 5 may be typical of low mass star-forming regions and chemical studies may reveal a great deal about dynamic processes occurring in them, but it is probably not representative of all dark clouds. However, a long term goal in molecular astrophysics is the construction of time dependent chemical models for realistic dynamical scenarios. Phil Myers has provided a review of the current state of knowledge of molecular cloud structure, dynamics, and evolution.

Part VI is primarily about infrared line emission from H_2 in regions of massive star formation. Tom Geballe has reviewed the observations. David Chernoff and Chris McKee have discussed shocks in dense molecular material. Most of the H_2 infrared emission in Orion comes from shock heated gas. David Neufeld has written about higher speed shocks which dissociate the molecules which pass through them and the chemistry in the postshock gas. Amiel Sternberg has described work on static ultraviolet induced dissociation regions which are also sources of H_2 infrared emission. Dense dissociation regions near bright stars can have H_2 infrared spectra which are similar to those originating in shocked gas.

Part VII concerns masers which are very near stars and the chemistry of gas in evolved stellar envelopes including supernova ejecta. Jim Moran's contribution contains discussions of the locations of OH, H_2O, and SiO masers relative to the central stars and the theory of radiative transfer in masers. Some astronomical masers are interstellar and are found very near young bright stars, while others are in the outflowing envelopes of highly evolved stars. Mike Jura has considered the chemistry in more expanded circumstellar envelopes around red giants. Dick McCray has reviewed what is known about the physical conditions in the ejecta of the supernova SN 1987A. A knowledge of those conditions is necessary for understanding the origin of and the relative concentrations of the molecules observed to exist in the ejecta. Detailed study of the chemistry in that environment is just beginning.

In Part VIII, Greg Shields has also written about processes in plasmas with temperatures around 10^4 K. In such plasmas thermal charge transfer, a process which one studies theoretically by first calculating the relevant molecular potential curves for the diatomic system and then solving the scattering problem, plays an important role in determining the ionization balance. Emission line regions in galaxies with active nuclei are amongst those sources in which charge transfer is important. John Black has described pregalactic chemistry and searches for molecular hydrogen in QSO spectra.

As editor, I am grateful to the contributors, all of whom have been cooperative and helpful.

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