PREFACE

On September 10, 2008, more than 125 friends, colleagues, and former students and postdocs gathered in Cambridge to join Professor Alex Dalgarno in celebrating his 80th birthday (which actually occurred on January 5, 2008). A symposium* highlighting Dalgarno's many scientific contributions was sponsored by the Institute for Theoretical Atomic, Molecular and Optical Physics (ITAMP) and held in Radcliffe Yard, September 10–12, and it included several receptions, a conference banquet, and closed with an evening concert in Cronkhite Courtyard.

Alex began his scientific career with a publication in the Proceedings of the Royal Society of London (1952). He has made seminal contributions in theoretical atomic and molecular physics, physics of planetary atmospheres and comets, molecular astrophysics, and astrochemistry. He has published nearly 750 peer-reviewed papers, conference proceedings and book chapters, including 7 papers in 2008. His average annual publication rate currently stands at 13. His most cited paper (*The Theory of Scattering by a Rigid Rotator*) published in 1960 with Arthurs has been referenced more than 935 times. He has five papers each with more than 500 citations. His h-index at 87 surely places him near the top of anyone's ranking, should he decide to leave Harvard for academic positions elsewhere.

Alex is clearly unique and his contributions have been wide-ranging, insightful, and influential.

The organizers of the Symposium—the editors of this book—intended the Dalgarno Celebratory Symposium to feature a range of topics representative of Alex's on-going scientific legacy and to be focused on his contributions over the last 20–25 years. The scientific program was divided into seven sessions.

The session on Calculations of Atomic and Molecular Properties was chaired by Ray Flannery. It reflected Alex's long-held belief that "Astrophysics is almost entirely applied Atomic, Molecular, and Optical Physics", and that to understand atomic and molecular reactions in astrophysical environments, one must first obtain an accurate picture of such processes through detailed and insightful calculations. Gordon Drake, in his review,

*http://www.cfa.harvard.edu/itamp/DalgarnoSymposium.html

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describes his work with Alex and later at the University of Windsor on the development of highly-accurate pseudospectral theory for the dipole response of atoms and molecules. Bernard Zygelman outlines the extension of Alex's successful spin exchange theory, based solely on the elastic approximation, to the collision of two spin-polarized hydrogen atoms, and its relation to the population of the hydrogen hyperfine levels, important in understanding emission or absorption of radiation in the 21 cm line. Michael Jamieson describes the current implementations of numerical techniques for the celebrated sum-over-all-state Dalgarno-Lewis method. Xi Chu supplies even more evidence for Alex's dictum, "the key to successful theoretical work is always to have more than one way of doing the same thing." She shows how to use the workhorse of theoretical chemistry—density functional theory (DFT)—to calculate the optical response of atoms and molecules.

The session on Astrochemistry was chaired by Bill Klemperer. The topic which Alex famously posed as a question in 1986, "Is Astrochemistry Useful?" was addressed by the four speakers in this session, each of whom offered an answer to that question. John Black pointed out that even in the Early Universe epoch of recombination, chemistry played a significant role, a point further emphasized by Phillip Stancil during his presentation of the H^- chemistry. Ewine van Dishoeck noted the myriad molecules which have thus far been detected and are archived on the web[†]. The review by van Dishoeck of the historical context and of Alex's seminal contributions to this interdisciplinary field is illuminating. Stephen Lepp writes about his experience working with Alex on the discovery of the molecular ions H_3^+ and HeH^+ in the spectra of the supernova remnant 1987A.

The session on the Interstellar Medium and Molecular Astrophysics resonated with the session on Astrochemistry. It was chaired by Pat Thaddeus. Tom Hartquist, in his review touches upon Alex's vast fundamental knowledge fueling his long term vision to construct detailed, robust models which can be applied to astrophysical environments. Reactions involving atomic deuterium allow for placing constraints on deuterium fractional ionization in dark molecular clouds, which in turn influences the role magnetic fields play in star formation in the dark clouds. The review describes how Alex recognized that HD was a much more effective coolant—due to its permanent dipole moment and its larger mass—than H_2, and the cooling rate increased with decreasing temperature. Amiel Sternberg describes Alex's insight in incorporating detailed molecular interactions (bond formation,

[†]http://www.astrochemistry.org

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bond destruction, and bond rearrangement) into quantitative interstellar cloud models. David Neufeld discusses the range of fine structure emissions from molecular ions, neutral molecule vibrational transitions, and rotational transitions of metal hydrides, all of which result from shock wave propagation in interstellar gases, and observation of interstellar hydrides using the Infrared Spectrograph on board the Spitzer Space Telescope. Cesare Cecchi-Pestellini—who unfortunately was not able to attend the Symposium—postulates that local turbulence thermal spikes may be responsible for the increased levels of H_3^+ and CH^+ in the diffuse interstellar medium.

The session on Atomic and Molecular Processes in the Solar System and Planetary Atmospheres, chaired by Jane Fox, was yet another example of the enormous breadth of Alex's research interests. Tom Cravens chronicles the many important contributions that Alex made to understanding the ionization, airglow, recombination and chemistry of planetary and cometary atmospheres. One important atomic process which regulates the radiation and heating in ionospheric plasmas is charge exchange between neutral species of interstellar or atmospheric origin and fast solar wind ions. This process, accompanied by emission of EUV or soft x-ray photons, is responsible for the x-ray radiation detected in cometary and planetary atmospheres and is described by Vasili Kharchenko in this volume. Peng Zhang describes his work with Alex on the thermalization path taken by hot atoms.

The session on Ultracold Collisions/Long-Range Interactions was chaired by Françoise Masnou. This session reflected Alex's more recent interest in cold collisions, but many of the collisional processes in ultracold physics have relied on Alex's seminal work four decades ago on the van der Waals and dispersive interactions between atoms, and between atoms and molecules. Using these ideas, important parameters for cold collisions, such as the *s*-wave scattering length, can be obtained from precise measurements of molecular transitions in ultracold regimes. Such processes are described in Randy Hulet's review of the field of photoassociation of ultracold atoms. Robin Côté's description of the formation of ultracold molecules by photoassociating two atoms at very large distances relies heavily on understanding the long-range atomic interactions and scattering information. Roman Krems writes about the development of numerical molecular basis representations for collisions involving molecules at cold temperatures and in the presence of external electrostatic fields. Very soon after the first atoms were cooled and trapped Alex began exploring the topic of cold molecular collisions and relaxation. He also has pioneered the study of reactions at

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ultracold temperatures, thus establishing the field of ultracold chemistry which Balakrishnan describes in detail.

Alex was available not only to his graduate students, postdocs or more senior fellows, but also to undergraduate students. Several of those who carried out undergraduate research projects with Alex and are now in graduate programs or in faculty positions described their work and their connections with Alex. The session was chaired by James Babb. In his contribution he discusses Alex's papers on the theory of the hyperfine structure of H_2^+ and some related studies carried out by several undergraduates working with Alex. Jean Turner, who studied under Alex as a junior and senior at Harvard (and now is a Professor of Astronomy at UCLA), gives an appreciation and discusses the frontiers of extragalactic astronomy. Ron Pepino was a visitor from the University of Connecticut and worked with Alex and Vasili Kharchenko for a few formative years starting with a summer visit. Now a graduate student in physics at University of Colorado-Boulder, he introduces the nascent field of 'atomtronics.' Jake Taylor started a project on the electronic structure of H_2^+ while a freshman at Harvard under Alex's guidance. After completing the project, and graduating, he went on to do his Ph.D. at Harvard with Mikhail Lukin. Presently a NIST Fellow, Jake discusses the theory and practice of magnetometry using diamond nitrogen vacancy centers and aspects of simulating quantum mechanical systems using optical lattices.

Alex was instrumental in bringing the Institute for Theoretical Atomic, Molecular, and Optical Physics to the Harvard-Smithsonian as an NSF-funded center. In his absence, ITAMP would not be where it is today. Many of the key players of the early and current days of ITAMP (Richard Pratt and Barry Schneider from the NSF and Kate Kirby from the CfA) offer historical perspectives on ITAMP and Alex's exceptional leadership in establishing this recognized institute which continues to thrive more than 20 years later.

Alex Dalgarno remains a towering figure in atomic and molecular physics and in astrophysics. The editors of this special edition focusing on his scientific legacy consider it an honor to be tasked with this historical endeavor and are grateful to Alex for his continued support and intellectual energy.

The organizers of this symposium are grateful for the support, including financial support, offered by the Harvard College Observatory and the Astronomy Department, in particular to Ms. Maureen Connors and Prof. Charles Alcock. We also thank Marion Shore for editing the concert program and several of the contributed papers. The local organizer, and the

person most responsible for ensuring the success of this symposium was Lisa Bastille, ITAMP Administrative Coordinator. The editors of this volume are indebted to her for her amazing organizational and diplomatic skills in coordinating the conference events and planning a memorable banquet at the Harvard Faculty Club.

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Kate Kirby
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Cambridge, MA
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