MOLECULAR HYDROGEN AND ITS IONS IN DARK INTERSTELLAR CLOUDS AND STAR FORMING REGIONS

by

Craig Alan Kulesa

A Dissertation Submitted to the Faculty of the

DEPARTMENT OF ASTRONOMY

In Partial Fulfillment of the Requirements
For the Degree of

DOCTOR OF PHILOSOPHY

In the Graduate College

THE UNIVERSITY OF ARIZONA

2002

STATEMENT BY AUTHOR

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Acknowledgments

I'd like to thank my advisor, J. J. Charfman, for...

Dedication

Nuclear war would really set back cable TV. –Ted Turner

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ABSTRACT

Fundamental observations of molecular hydrogen (H_2) in dark clouds, star forming regions, and radiation–dominated environments are presented, modeled, and interpreted. Through a weak infrared absorption line spectrum, the abundance of cold H_2 in dark molecular clouds and star forming regions is measured directly and compared with the abundance of its most commonly cited surrogate, CO. The derived abundance of CO is between 1.5 and 2.5 $\times$ 10^{-4} for the sample. The CO molecule thus represents about $^1/_3$ of the total carbon budget in dense clouds. Also detected via infrared line absorption is the pivotal molecular ion H_3^+, yielding a direct measure of the cosmic ray ionization rate of H_2 in dark molecular clouds (between 1 and 5 $\times$ 10^{-17} s^{-1}), a process that instigates the complex ion-neutral chemical pathways that form many of the 120+ known molecular species deep inside interstellar clouds. These timely tests of theory are applied to the detailed submillimeter–wave study of the ρ Ophiuchi star forming cloud and photodissociation front, allowing partial disentanglement of the complicated physical and chemical structure of a star forming cloud. Yet H_2 and H_3^+ continue to surprise and delight us with more mysteries. The formation, excitation and survival of molecules in unusual & hostile environments is highlighted by the discoveries of H_3^+ in circumstellar disks of early–type stars, and of fluorescing H_2 in two harshly–irradiated filaments of the Crab Nebula. The role of H_3^+ as a possible tracer of planet formation, and the evolution of H_2 in the interstellar medium is discussed. The study of H_2 in hostile environments is extended to the ensemble properties of extragalactic star forming regions, and applied to the Arp 299 merger system as a unique probe of the feedback of newly-formed hot stars, their fossil remains, and the molecular material which formed them.

CHAPTER 1

INTRODUCTION

I write about molecules with great diffidence, having not yet rid myself of the tradition that atoms are physics, but molecules are chemistry, but the new conclusion that hydrogen is abundant seems to make it likely that the above-mentioned elements H, O, and N will frequently form molecules.

Sir Arthur Eddington (1937)

Recognition of the existence of interstellar molecules and their importance to all aspects of astrophysics has reached a critical mass. The humble beginnings of astrochemistry, marked by the detection of interstellar CN, CH and CH^+ absorption lines at visible wavelengths toward background stars in the late 1930's, have given way to a renaissance of discovery and the formation of an interdisciplinary field, astrochemistry, whose grasp reaches from comets to cosmology, from meter-wave radio wavelengths to X-rays, from simple diatomic molecules to organic species approaching the complexity of amino acids, in environments ranging from cold and quiescent to violently hostile and dynamic. It is now well accepted that molecular interactions, both with radiation and each other, provide a unique observational and theoretical tool of unprecedented diagnostic power. It is less often realized that the mere existence of molecules, through their pivotal effects on their environment's ionization and thermal balance, can strongly regulate their dynamical and chemical evolution. Indeed, exploration and definition of this facet of molecular astrophysics may well be its ultimate contribution to the whole of astrophysics.

1.1 Importance of H_2 and its ions H_2^+ and H_3^+

Theoretical and observational evidence has established that 90 percent (by number) of the known baryonic matter in the Universe is composed of elemental hydrogen (Boesgaard & Steigman, 1985; Peebles, 1993). The astronomer's periodic table is therefore an unusual sight to traditional physicists and chemists (Figure 1.1). Therefore, of the 123 interstellar molecules reported to date (Wootten, A., 2002), it is fully expected that the hydrogen molecule (H_2) is by far the dominant constituent of astrophysical plasmas. Indeed, the contribution of H_2 to the total baryonic mass of the Universe is predicted to be secondary only to atomic hydrogen, helium, and their ions. Furthermore, molecular hydrogen has the unique and pivotal distinction of being the gaseous state of hydrogen that gives rise to the formation of stars.

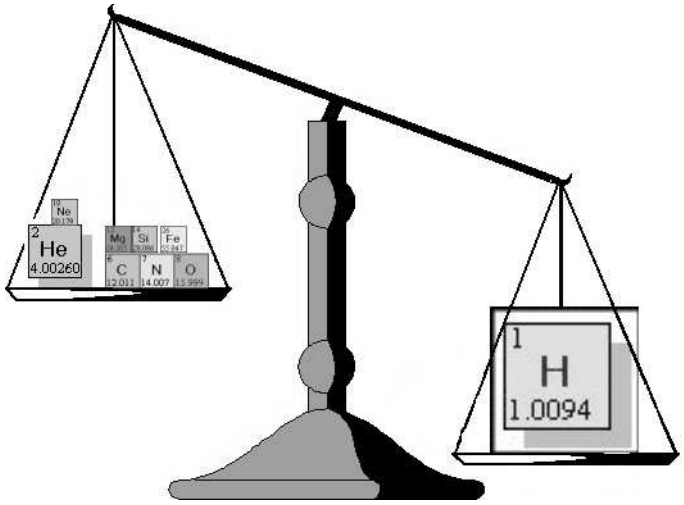

Figure 1.1: Weighing the elemental universe. Big Bang nucleosynthesis formed hydrogen, helium, and a small amount of lithium. 10^{10} yr of stellar evolution and enrichment of the interstellar gas has added carbon, nitrogen, oxygen, magnesium, silicon and iron to the scales, in addition to trace amounts of numerous other species – but hydrogen still outweighs them all.

Interstellar gas is continuously replenished by the final phases of stellar evolution, principally the mass loss of asymptotic giant branch (AGB) stars and envelope ejection of supernovae explosions (Spitzer, 1978). The conversion of interstellar gas from atomic to molecular form depends primarily upon sufficient gas and dust density and the strength of the ambient interstellar radiation field. The phase transition from atomic to molecular gas in interstellar clouds is sharply defined, generally dictated by radiative processes, and hence described as a photon-dominated region, or photodissociation region (PDR) (Tielens & Hollenbach, 1985; Black & van Dishoeck, 1987; Draine & Bertoldi, 1996). Not only does H_2 dominate the mass of such molecular clouds, but the thermal balance of its formation energy and emission of radiation at infrared wavelengths plays a significant role in the physical state and evolution of such clouds. Indeed, the formation of all stars from dense condensations in molecular clouds gives H_2 special importance in the complicated symbiosis of the interstellar medium (ISM) of the Galaxy and the stars that form from it. As primordial species in the gas dominated post-recombination Universe, H_2 provided new mechanisms of heating and cooling which played a role in the formation of the very first star forming structures which led, either eventually or contemporaneously, to the formation of the first galaxies (Anninos & Norman, 1996; Norman & Spaans, 1997; Haiman, Abel, & Rees, 2000; Hutchings, Santoro, Thomas, & Couchman, 2002). The critical role of H_2 as star-forming fuel therefore has significant cosmological implications.

The role of the ions derived from H_2 are no less important. The ionization of H_2 by photons of energy 15.4 eV or greater, most typically by the local production of X-rays and energetic cosmic rays, results in the creation of H_2^+. H_2^+ is very short lived in the interstellar medium, reacting with nearly every collision partner it encounters. In dense molecular clouds, the most probable reaction is with H_2, re-

sulting in the production of H_3^+ (Martin, McDaniel, & Meeks, 1961), which in turn represents the cornerstone of the gas phase reaction networks that initiate the formation of most other molecules in interstellar space (Figure 1.2). In the absence of ultraviolet (UV) radiation in the dark interiors of molecular clouds, the H_2 ionization rate therefore defines the energetic chemical processes that form most other molecules (Herbst & Klemperer, 1973). Therefore, the measurement of H_3^+ in concert with H_2 represents the most direct confirmation of the gas phase production of molecules by measurement of the cosmic ray ionization rate of H_2 that initiates these chemical networks. Similarly, H_2^+, H_3^+ and their daughter ions partially control the ionization fraction in molecular clouds, which in turn regulates the ability of a molecular cloud condensation to withstand self-gravitational collapse to form new stars and planets due to interaction with magnetic fields. Owing to their relative simplicity among molecules, H_2, H_2^+ and H_3^+ also represent our best theoretical models of the quantum mechanical structure of molecules, and the subsequent spectroscopic tests of such theories in both Earth-based and interstellar laboratories have an important, ongoing history.

Okay, that's enough. I quit. :)

But first, here's a random table!

Table 1.1. Thermalized H_2 line emission

T(K)	$I_{S(0)}$	$I_{1-0\ S(1)}$	I_{tot}
10	5.9248e-25	0.0	5.9248e-25
20	6.9748e-14	0.0	6.9748e-14
50	2.3665e-07	0.0	2.3774e-07
100	1.8863e-05	0.0	3.2499e-05
150	6.7871e-05	9.9590e-18	3.4086e-04
200	1.2315e-04	8.1477e-13	1.3739e-03
300	2.1476e-04	6.0481e-08	7.5244e-03
500	3.2295e-04	3.9785e-04	6.2136e-02
1000[b]	4.2691e-04	2.1145e-01	2.1839e+00
2000[b]	4.8601e-04	3.3212e+00	3.9504e+01
3000[b]	5.0667e-04	6.7842e+00	2.2498e+02

[a]All intensities in erg s^{-1} cm^{-2} sr^{-1} for a $N(H_2)= 10^{22}$ cm^{-2} thick plane-parallel slab

[b]High temperatures are likely to only apply to the surfaces of interstellar clouds, not to an entire "dark" cloud

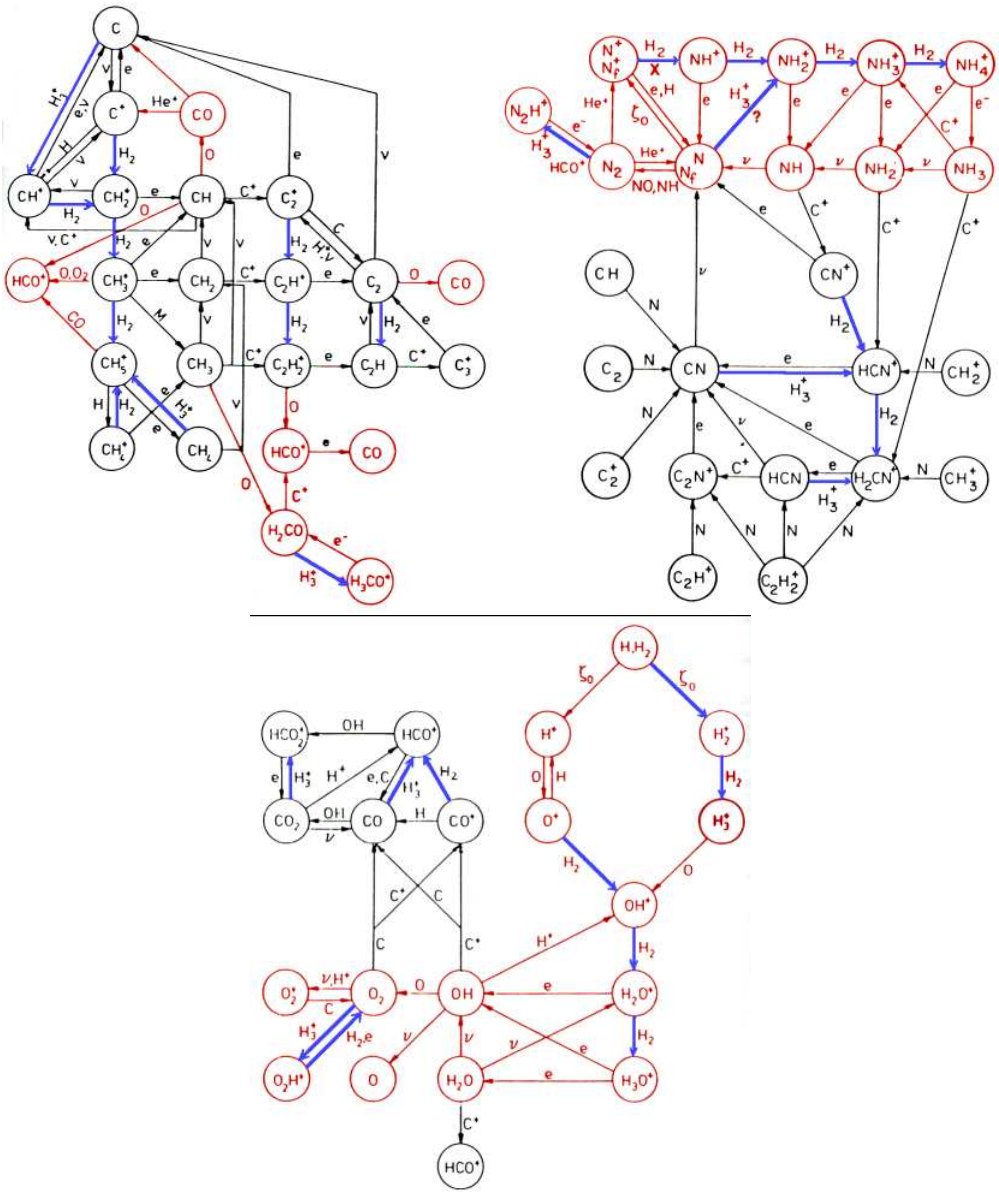

Figure 1.2: Simplified chemical networks for carbon (overlap with oxygen in red), nitrogen (overlap with carbon in red) and oxygen (overlap with carbon in red), adapted from Prasad, Tarafdar, Villere, & Huntress (1987). The role of H_2 and H_3^+ as the initiators of the gas phase chemistry in each network is highlighted in blue bold strokes.

CHAPTER 2

DIRECT MEASUREMENT OF MOLECULAR HYDROGEN AND ITS IONS IN INTERSTELLAR CLOUDS AND STAR-FORMING REGIONS

Unfortunately, because they are mostly composed of molecular hydrogen (H_2) and also because they are so cold, 99% of a molecular cloud's mass is virtually undetectable by means of direct observations.

ESO Press Release 29a-c/99

To date, over 120 different molecules have been detected in the interstellar medium, and some, such as the common molecular ion HCO^+, have been identified in space before being synthesized on Earth. Through their spectra, these interstellar molecules provide a wide range of diagnostic probes of conditions in molecular clouds and star-forming regions; through their interactions with radiation and with each other, they also partly regulate the dynamical evolution of interstellar clouds.

Although most interstellar molecules have been detected through emission line spectroscopy at millimeter wavelengths, this technique is inapplicable to non–polar molecules like H_2, CO_2, C_2H_2, and H_3^+, which are thought to be central to our understanding of interstellar chemistry. In particular, H_2 comprises the vast majority of the mass in star–forming molecular clouds, a large fraction of the interstellar mass of the Galaxy, and plays a significant role in the heating and cooling, and hence *evolution* of interstellar gas. All stars, as far as we know, are born from dense, dark molecular clouds whose hydrogenic contents

are composed almost entirely of H_2. The role of protonated H_2, H_3^+, is no less significant. H_3^+ is the cornerstone of interstellar chemistry responsible for initiating the gas-phase chemical networks that form many of the observed molecules in dark clouds (Herbst & Klemperer, 1973; Watson, 1976). H_3^+ forms from H_2 by the cosmic ray ionization of H_2 to H_2^+:

$$H_2 + \text{c.r.} \rightarrow H_2^+ + e^- \tag{2.1}$$

$$H_2^+ + H_2 \rightarrow H_3^+ + H \tag{2.2}$$

The first reaction is slow; a typical H_2 molecule in the ISM will be ionized once every billion years. Once H_2^+ forms however, only 10^5 seconds elapses before it reacts with the first available species, typically another H_2 molecule. Thus, the ionization of H_2 results in the efficient and rapid production of H_3^+. Measurement of H_3^+ provides the most direct measurement of this fundamental process that initiates chemical models of interstellar clouds and star forming regions.

The physical symmetry of H_2 and H_3^+ give them vanishingly small permanent dipole moments and therefore do not allow for a traditional rotational emission line spectrum at radio wavelengths. Hopes for detecting the dominant H_2 molecule in cold clouds are frustrated further by its low moment of inertia, which yields large rotational energy level spacings that are energetically unreachable to cold hydrogen molecules in molecular clouds (see Introduction). Direct measurements of H_2 in its ortho- and para- ground states are made possible by a dipole-permitted electronic absorption line spectrum in the vacuum ultraviolet between 912 and 1130 Å. Although such observations, made possible by space-borne telescopes like *Copernicus* and FUSE, are critical to assessing the chemistry and contents of diffuse clouds, they are inapplicable to studies of the dense, dark

clouds where stars are formed. Thus, indirect measures of the abundance of H_2 have been necessary.

Okay, that's enough of that. Get the idea? :)

APPENDIX A

A GUIDE TO REDUCING DATA TAKEN WITH THE PHOENIX INFRARED SPECTROMETER

This document is available online in browsable (color) format at:

`http://loke.as.arizona.edu/~ckulesa/phoenix/reduction/`

A.1 Introduction

Phoenix is a cryogenic, long slit, high resolution infrared spectrograph designed for use at the f/15 focus of the KPNO 2.1-meter, the KPNO, CTIO and SOAR 4-meter, and the Gemini 8-meter telescopes. For more instrument details, consult the Phoenix Web Page and the Phoenix Instrument Manual.

This document graphically describes the data reduction process, following the reduction of a complete dataset to a publishable result, and includes a Phoenix IRAF package containing tasks to speed along the data reduction process. It documents a method of data reduction which is robust and highly optimized for getting the most from Phoenix data. It is certainly not the only way, but it should save you a lot of time. If you find a way to improve the techniques provided here, I want to know!

It is designed to complement the NOAO data reduction exercise, which nicely covers general aspects of spectroscopic reduction in IRAF, but not the more spe-

cific issues of IR data reduction as pertains to Phoenix data. For example, successful reduction of pre-2001 Phoenix data (with the old Aladdin I array) critically hinges upon careful bad pixel rejection and image combination, which isn't discussed at all.

This exercise uses a basic installation of IRAF, the Image Reduction and Analysis Facility (some say, It Reeks And Fumes), although new reduction pipelines that operate independently of IRAF (using PDL and Python) are in development. Until such pipelines are completed, basic IRAF functionality is necessary.

A.2 Outline of the Basic Steps for Phoenix Data Reduction

- Make IRAF go
- Combine Dark Frames `[imcombine]`
- Construct Flat Field Frame:
  - Combine flat field frames `[imcombine]`
  - Subtract dark frame `[imarith]`
  - Normalize image to unity `[imarith]`
  - Correct for spectral response `[response]`
- Selecting Files for Bulk Processing
- Sky-subtract, Flat-field + Trim data frames `[phxproc]`
- Combining frames:
  - Squashing images to measure offsets `[squash, splot]`
  - Expanding and aligning images `[strexp, nalign]`

  - Combining frames, removing spectral tilt & bad pixels `[mask, ircombine]`
  - Contracting images to original scale `[contract]`

- Extraction of 1D spectra: `[apall]`
  - Defining apertures `[apedit]`
  - Tracing spectra `[aptrace]`
  - Extraction and 2nd pass at removing bad pixels `[apextract]`
  - Reviewing your spectrum `[splot]`
- Telluric Correction `[telluric]`
- Wavelength Calibration `[identify, refspec, dispcor]`
- Getting Data out of IRAF `[wspectext]`

A.3 About the Spectra used in this Tutorial

We will be processing data taken after the clearing of monsoon storms on the morning of 2000 July 16, at the venerable Kitt Peak 2.1-meter telescope. The data is of a heavily-embedded young stellar object S140 IRS 1 in the L1204 molecular cloud (Cepheus). It is a 7th magnitude source at the 2.34 micron (4272 cm^{-1}) wavelength of the R-branch of the first overtone ^{12}CO band. Owing to the high degree of obscuration, we expect to see the signature of interstellar CO absorption lines along this line of sight. We are using the spectrum of Deneb (which was at a similar elevation at the time of observations) as a comparison spectrum to remove atmospheric features. The data are composed of eight 600-second exposures, with "seat of pants" guiding as this source is optically invisible. Slit losses due to inaccurate guiding are estimated to be 20-30%; pretty good considering! Note

that these data were taken with the "old" *Aladdin I* array, and with multiple-sampling (i.e. 4 Low Noise Reads), about 5% of the array's pixels are bad and must be discarded. This dataset therefore represents an instructive challenge, as improper rejection of bad pixels will yield useless results.

Below is an image of S140 IRS 1 at 2.34 microns, taken with Phoenix in imaging mode during target acquisition.

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