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Astrochemistry - April 2008

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Professor Tom Millar
From the Special Topic of Astrochemistry

The physics and chemistry of star formation is played out in dense interstellar clouds, which are the nurseries of new stars, together with their attendant proto-planetary disks, from which planets condense. The discipline that considers the formation, interaction, and destruction of molecules in space is astrochemistry. Its importance has increased considerably with the explosive growth of astrobiology and the attendant quest to understand the molecular origin of life in the universe. The use of astrochemical models to interpret molecular line observations is widespread.

A Special Topics examination of astrochemistry research over the past decade highlights the contributions of Professor Tom Millar, who ranks at #1 by cites/paper, #3 by cites, and #9 by number of papers, with 14 papers cited a total of 534 times. Two of these papers rank at #2 and #4 respectively on our list of the 20 most-cited papers in the field.

Professor Millar is Dean of the Faculty of Engineering and Physical Sciences and Professor of Astrophysics in the School of Mathematics and Physics at Queen’s University, Belfast, in Northern Ireland.

In the interview below, Dr. Simon Mitton, ScienceWatch.com's *European correspondent, interviewed Professor Millar to find out more about his high-ranking papers related to astrochemistry*.

SW: I picture chemistry as an industrial enterprise, with its intellectual puzzles normally being pursued in laboratories. But you are an exception to this simplistic view because your interests are the chemical reactions that take place in space, in environments where the physical conditions, particularly densities, temperatures, and time scales could scarcely be more different than in the laboratory. How did you get into such an esoteric field?

I attended the University of Manchester Institute of Science and Technology (UMIST) where I read mathematics, staying on to do a Ph.D. with David Williams in astrophysics. In practice though, my doctoral research was in the field we now term astrochemistry; I was probably the first person to get a Ph.D. in astrochemistry from a UK university.

My thesis looked at molecule formation in interstellar clouds. Back in the mid 1970s, new interstellar molecules were first being discovered through techniques of microwave radio astronomy. Everyone got tremendously excited by the discoveries of ammonia (NH_3) and formaldehyde (H_2CO), the latter a central building block in the synthesis of many other compounds.

SW: I well remember that excitement: I was a graduate student in radio astronomy at Cambridge, although my interests were certainly not on the molecular scale because I was observing quasars and radio galaxies.

It was indeed a most stimulating time, and I started working on models of how those interstellar molecules could form. I did some work on investigating the importance of various gas-phase mechanisms on molecule formation. A big chunk of my thesis was on numerical modeling of cloud collapse with molecule formation included. By the time I finished I felt I knew as much as one could then about molecules and gaseous chemistry, but I knew very little about interstellar dust, which is important in astrochemistry because molecules freeze onto the dust at very low temperatures.

I went off to be a postdoc in Toronto with Walt Duley, who had done a lot of work on interstellar dust; I wanted to learn from him how to study dust, particularly its optical and physical properties. I was interested in how dust could protect molecules from strong radiation, which would destroy them, and I was also interested in surface chemistry. From Toronto I went to Oxford as a postdoc, thence to an appointment as a lecturer in mathematics at UMIST, before moving to Queen’s University here in Belfast.

> *"What my research is all about is trying to use molecules as tracers of the history of molecular clouds."*

SW: What are your current interests? I note that you are currently Chair of the International Board of the James Clerk Maxwell Telescope (JCMT) in Hawaii and that you are serving as President of Division VI (Interstellar Matter) of the International Astronomical Union.

The underlying theme that interests me is the use of chemistry of molecules as probes of the physical conditions in interstellar space. To me that’s more than a question of using molecules as proxies to get temperatures, densities, the strength of magnetic fields and so on. What my research is all about is trying to use molecules as tracers of the history of molecular clouds.

SW: Are giant molecular clouds, of a million solar masses or more, the most important sites for star formation?

They certainly are. An important aim at which I have been working hard to understand for several years is: what are the best molecular probes of the star formation process? One of the big problems in star formation is the transition from an interstellar cloud that has relatively low density and is cold, to a protostar, in which the nuclear fusion processes can commence. And if you try to follow the physical conditions theoretically you find you get to a stage where the gas is dense but still cold—10 K.

At those temperatures everything sticks to the dust on timescales of hundreds of years, much shorter than the time scale of star formation. Molecules such as carbon monoxide or ammonia, which astrochemists and radio astronomers use to probe physics, have frozen out and have ceased to be applicable as probes. With the molecules frozen out the only components of the gas are hydrogen, deuterium, and helium, and they form very few observable species, such as H_2D+ and D_2H+, but in surprisingly high abundance.

SW: Are your interests today are broader than just the theoretical side of the astrochemistry of molecular clouds?

You bet. I apply astrochemistry to a whole variety of environments such as interstellar clouds, protoplanetary disks, planetary nebulae, late-type stars, masers, and models for molecular clouds in external galaxies. I have an observational program as well that uses molecules to trace what’s actually happening in the process of star formation. I’ve also put in place an observational program that allows us to test our own models. To do so we use the JCMT and other radio and submillimeter telescopes around the world. I also work very closely with scientists who are doing laboratory studies on reaction rates. Indeed one of the pleasures of working in this field has been the interdisciplinary nature of the research.

SW: Your two most-cited papers are for the 1995 and 1999 editions of the UMIST databases for astrochemistry (Millar TJ, *et al., Astron. Astrophys. Suppl*. 121:139-85, 1997 and Le Teuff YH, *et al., Astron. Astrophys. Suppl*. 146: 157-68, 2000, respectively). The results of those compilations are clearly much in demand. How did the project start?

When we first started working on the chemistry of interstellar clouds, my group was doing cutting-edge research, but we were finding that there were few groups around with whom we could interact. The fundamental data for our models are chemical reaction rates. We have spent many years building this from a variety of sources. Importantly for the science, we had a tough time trying to convince observers to run tests for our models. So we decided to make all of our computer code and our data available to the community worldwide, so that the observers could develop models and see that they are of value in understanding interstellar physics.

SW: The first edition was published in 1991. By going public your group had, to a large extent, taken a calculated risk for the public good that you would still have plenty of research to do on refining your models. How did publication affect the citation rate?

> *"ALMA will be able to peer in detail at star-formation regions in molecular clouds."*

The publication of the UMIST databases and the computing codes to go with them was not a decision that we took lightly. We had a long argument within our group about whether it's best to keep your codes and data private. The advantage of non-disclosure is that you can keep your research cutting edge because you possess some tools that none of your competitors have. You can get your papers published quickly without competition. On the other hand, we could make everything available to the world and then have to live with the competition that comes from other people using our codes and having better ideas.In the end we decided that it would be better for the project as a whole and better for us—we had to have the confidence to remain competitive in an even more competitive world—if we simply made everything public. So that's the publishing story underlying our most highly cited papers.

By going that route we have stimulated far more groups, internationally, to take an interest in astrochemistry. It has meant that observers can do their own modeling to interpret the observations, and that has to be a good thing. We published the first version back in 1991, and we release updated versions about every 4–5 years. The 2006 database was released in June 2007.

SW: The 2006 database (Woodall J, *et al., Astron. Astrophys*. 466:1197-U203, 2007) is already ranked #7 in citations of your papers. What's new in this version?

The current version contains some 4,573 binary gas-phase reactions, an increase of 10% from the previous (1999) version, among 420 species, of which 23 are new to the database. We have made updates to ion-neutral reactions, neutral-neutral reactions, particularly at low temperature, and dissociative recombination reactions. We have included for the first time the interstellar chemistry of fluorine. Everything is available at http://www.udfa.net/.

SW: The high citation level suggests that these papers are appealing to a broad audience.

That's right. In addition to the astrochemistry, we get a lot of citations from atmospheric physics. Also we get citations from astrobiologists looking at the chemistry of the early solar system. Furthermore, the combustion and fusion communities use our data.

SW: I notice you have a cluster of highly cited papers on deuterium fractionation in molecular clouds.

The D/H ratio at the end of the Big Bang was about 10^{-5}. However, since the mid-1970s observers have been finding D/H ratios of 1% in interstellar molecules, which represents an enhancement by a factor of 1,000. When we started to model this effect we found that because of the fact that deuterated molecules have lower zero-point energies than their hydrogenated form, they get formed preferentially at low temperatures. We found that a D/H ratio of 1% could be reached in an interstellar cloud at a temperature of 10K, such as the dense cloud in Taurus.

In more recent years when people have been using radio interferometers to look at star formation regions they started finding out that some of the D/H ratios were very large, and they found multiply deuterated molecules. Most spectacularly, triply deuterated ammonia was 10^{12} times more common than the raw statistics would suggest.

Our papers look at the physical conditions required to get these enormous enhancements. What we found in the series of papers is that in regions of cloud where the matter density is about 1000 times higher than the average, but still at a temperature of 10 K, everything but hydrogen and deuterium freezes. This leads to very large enhancements in deuterium fractionation in the gas phase and, through collisions with the dust grains, to an ice chemistry in which deuterated molecules are made very efficiently.

SW: Finally, let's look at where your research is now headed. The Atacama Large Millimeter Array (ALMA) is one of the largest ground-based astronomy projects. When completed in 2012, this major new facility will surely impact on observational astrochemistry.

This is a very exciting time for astrochemistry. ALMA will have unprecedented spatial resolution, frequency coverage, and sensitivity for the study of molecular emission. We are trying to make predictions for what ALMA might see in very small, cold, star-forming regions or protoplanetary disks. We're also interested in the connection between the early solar system and the interstellar gas. ALMA will be able to peer in detail at star-formation regions in molecular clouds. ALMA should get plenty of data to challenge our models and the laboratory studies we have on hand.

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Professor Tom Millar's most-cited paper with 152 cites to date:

Le Teuff, Millar TJ, Markwick AJ, "The UMIST database for astrochemistry 1999," *Astron. Astrophys. Suppl. Series* 146(1): 157-68, October 2000. Source: *Essential Science Indicators*SM from Thomson Reuters.

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