WINTER 2003

Miller Institute News

The Miller Institute is "dedicated to the encouragement of creative thought and the conduct of research and investigation in the field of pure science and investigation in the field of applied science in so far as such research and investigation are deemed by the Advisory Board to offer a promising approach to fundamental problems."

Miller Fellow Focus: Ben McCall

Second year Miller Fellow Ben McCall works across the disciplines of physical chemistry and molecular astrophysics. He is hosted by Professor Richard Saykally in the Department of Chemistry, but also collaborates with James Graham in the Department of Astronomy.

The multidisciplinary nature of McCall's work is illustrated by his research on the H_3^+ molecular ion. This ion is the simplest polyatomic molecule, as it consists of only three protons bound together by just two electrons. This non-classical molecule is stable in the absence of collisions but is an incredibly strong acid: that is, it will quickly donate its "extra" H^+ to just about any other atom or molecule. This extreme chemical reactivity makes H_3^+ a key player in the chemistry of interstellar space.

The space between the stars is not completely empty; although the average density is very low (about 1 atom or molecule per cubic centimeter), there are numerous "interstellar clouds" where the densities are considerably higher. These clouds are generally divided into two groups: "dense clouds," which are held together by their self-gravity and serve as the birthplaces of stars, and "diffuse clouds," whose evolutionary role is less clear. In dense clouds, H_3^+ dominates the chemical scene and is responsible for the production of nearly all of the observed molecules, including the water that eventually found its way to Earth.

The concentration of H_3^+ in an interstellar cloud can be estimated by equating the rates of its formation and destruction. The formation of H_3^+ is precipitated by the impact of a cosmic ray with a hydrogen molecule to form H_2^+, followed by the fast reaction $H_2^+ + H_2 \rightarrow H_3^+ + H$. In dense clouds, the dominant destruction pathway of H_3^+ is a chemical reaction with carbon monoxide: $H_3^+ + CO \rightarrow HCO^+ + H_2$ (this is an example of H_3^+ acting as an acid). While the formation pathway of H_3^+ is the same in diffuse clouds, the destruction is dominated by the much

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faster reaction $H_3^+ + e^- \rightarrow 3H$ (because diffuse clouds are less dusty, starlight can penetrate them and ionize atoms like carbon, leaving abundant electrons). Since H_3^+ is formed at the same rate but destroyed more quickly, it was thought to be very much less abundant in diffuse clouds.

As a graduate student at the University of Chicago, McCall (along with his thesis advisor Takeshi Oka and collaborators Tom Geballe of Gemini Observatory and Ken Hinkle of the National Optical Astronomy Observatories) measured the amount of H_3^+ in dense interstellar clouds, using the United Kingdom Infrared Telescope (UKIRT) in Hawaii and the 4-meter telescope at Kitt Peak National Observatory in Arizona. These observations were consistent with the simple chemical model described above, and confirmed the central role of H_3^+ in dense cloud chemistry.

However, McCall and his team were in for a shock when they turned their telescopes to diffuse clouds — the H_3^+ absorption lines there were just as strong as in dense clouds! Because the spectrum measures the total number of ions along the line of sight (i.e. the concentration times the path length), this implied a very long path length if the chemical model was to be believed. So long, in fact, that nearly all of the distance between the Earth and the stars used as light sources for the absorption measurements must be filled with diffuse cloud H_3^+!

The chemical model used to infer the H_3^+ concentration in diffuse clouds has only four parameters: the rate of the $H_3^+ + e^-$ reaction (k_e), the cosmic ray flux (ζ), the ratio of electrons to hydrogen molecules (f), and the size of the cloud (L). The first of these (k_e) is a universal rate constant, and can be measured in the lab — however, all of the measurements to date have used H_3^+ ions at room temperature or hotter, whereas diffuse clouds are much colder (~30 K).

In collaboration with Saykally, Berkeley graduate student Alex Huneycutt, and recent Visiting Miller Professor Mats Larsson (Stockholm University), McCall set out to make a measurement of k_e that would be more applicable to diffuse clouds. The idea was to create the H_3^+ ions in a flow of H_2 molecules expanding through a small pinhole from a high-pressure region (~2 atmospheres) into high vacuum. In such a supersonic expansion, the initial random motions of the gas are converted into a directed flow, resulting in a very low temperature. Such sources are routinely used for molecular spectroscopy, but had never been applied to rate constant measurements.

The source was constructed in Berkeley and characterized using the high sensitivity technique of cavity ringdown laser absorption spectroscopy in the Saykally lab. By directly measuring the spectrum of H_3^+ in this source (the same spectrum that is observed in interstellar space!), the low temperature of the ions was confirmed. McCall and Huneycutt then took the source to Stockholm and mounted it on the ion-storage ring CRYRING. There, the cold H_3^+ ions could be accelerated and stored for tens of seconds in a particle accelerator, and merged with a beam of cold electrons, yielding a direct measurement of k_e under conditions closely mimicking diffuse clouds.

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Miller Fellow Benjamin McCall

Recent Publications

Miller Professor Paul Alivisatos (Academic Year 2001-2002) had a prolific Miller Professorship term publishing numerous papers including, "Less is More in Medicine," Scientific America, 285, N3:59-65 (September 2001) and "Activation Volumes for Solid-Solid Transformations in Nanocrystals," with K. Jacobs, D. Zaziski, E.C. Schner, and A.B. Herold, Science, 293, 1803 (September 2001). Professor Alivisatos also published an additional fourteen papers.

Miller Professor Martin Head-Gordon (Academic Year 2001-2002) published three papers during his Miller term: "Fast evaluation of a Linear Number of Local Exchange Matrices," with W.Z. Liang, Y. Shao, C. Ochsenfeld, and A.T. Bell, Chem. Phys. Lett. 358, 43-50 (2002), "Can coupled cluster singles and doubles be approximated by a valence active space model?" with G.J.O. Beran, and S.R. Gwaltney, J. Chem. Phys. 117, 3040-3048 (2002), and "Quadratic coupled-cluster doubles: implementation and assessment of perfect-pairing optimized geometrics," with E.F.C. Byrd, and T. Van Voorhis, J. Phys. Chem. 106, 8070-8077 (2002).

Miller Professor Jitendra Malik (Fall '01) published one paper during his Miller Professorship: "A Probabilistic Multi-scale model for Contour Completion Based on Image Statistics," with X. Ren, Proc. of 7th ECCV, May 2002, Vol. 1. Springer LNCS 2350, pp. 312-327.

Miller Professor Paul Richards (Fall'01) published one paper during his Miller Professorship: "Tests for Gaussianity of the MAXIMA-1 CMB Map," with J.H.P. Wu, A. Balbi, J. Borrill, P.G. Ferreira, S. Hanany, A.H. Jaffe, A.T. Lee, B. Rabii, G.F. Smoot, R. Stompor, and C.D. Winant, Phys. Rev. Lett. 87, 251303 (2001).

Miller Fellow Venkatesan Guruswami ('01-'02) published two papers during his Miller term: "Combinatorial bounds for list decoding," with H. Hastad, M. Sudan and D. Zuckerman, IEEE Transactions on Information Theory, 48(5): 1021-1035, May 2002, and "Reflections on Improved decoding of Reed-Solomon and Algebraic-geometric codes," with M. Sudan, IEEE Information Theory Society Newsletter, Volume 52, Number 1, ISSN 1059-2362, pp 6-12, March 2002.

Miller Fellow David Keys ('99-'02) published two papers during his Miller term: "Genome-wide identification of tissue-specific enhancers in the Ciona tadpole," with N. Harafuji and M. Levine, Proceedings of the National Academy of Sciences, USA, 99:6802-6805 (2002), and "Control of intercalation is cell-autonomous in the notochord of Ciona intestinalis," with M. Levine, R.M. Harland and J.B. Wallingford, Developmental Biology, 246:329-340 (2002).

Miller Fellow Yasunori Nomura ('01-'02) had a productive term with the Miller Institute: "Gauge-Higgs Unification in Higher Dimensions," with L. Hall and D. Smith, Nucl. Phys. B639, 307 (2002), and "R Symmetry and the ì Problem," with L.J. Hall and A. Pierce, Phys. Lett. B538, 359 (2002). Dr. Nomura published an additional seventeen papers.

Miller Fellow Steven Poe ('00-'02) published two papers during his Miller term: "Character selection and the methodology of morphological phylogenetics," with J. J. Weins, Phylogenetic Analysis of Morphological Data (J.J. Weins, ed.), pp 1-26 (2000), and "Philosophy and phylogenetic inference: A comparison of parsimony and likelihood methods in the context of Karl Popper's writings on corroboration," with K. De Queiroz, Systematic Biology 50:305-321.

MILLER RESEARCH PROFESSOR AWARDS

The Miller Institute is pleased to introduce the 2003-2004 Miller Research Professors. The Executive Committee and Advisory Board of the Miller Institute have granted awards to the following Berkeley professors for appointments during the 2003-2004 academic year.

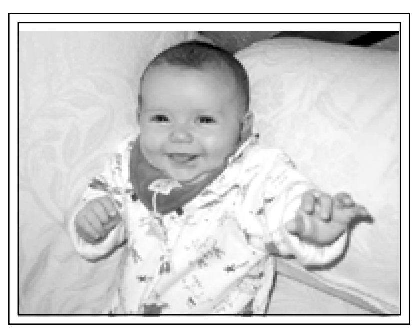
Astronomy	Professor Imke de Pater
Chemistry	Professor Judith Klinman
Earth & Planetary Science	Professor Lynn Ingram
Electrical Engineering & Computer Sciences	Professor Connie Chang-Hasnain
Integrative Biology	Professor Ellen Simms Professor Montgomery Slatkin
Materials Science & Engineering	Professor Daryl Chrzan
Mechanical Engineering	Professor Arunava Majumdar
Molecular and Cell Biology	Professor George Oster
Statistics	Professor Bin Yu

The Stork Club

The Miller Institute would like to congratulate third year Miller Fellow Yann Capdeville and his wife Betty Capdeville on the birth of their second daughter Léane.

Léane was born on September 7, 2002.

Léane and Laurine Capdeville



Léane Capdeville

VISITING MILLER PROFESSOR AWARDS

The Executive Committee and Advisory Board of the Miller Institute have granted awards to the following Visiting Miller Professors. Their terms range from thirty days to one semester during the 2003-2004 academic year.

Astronomy	Professor Avishai Dekel, The Hebrew University, Jerusalem Professor Norman Murray, University of Toronto, Canada
Chemical Engineering/MCB	Professor Alan Perelson, University of California, Los Alamos National Laboratory, New Mexico
Chemistry	Professor Odile Eisenstein, Universite Montpellier, France Professor Paul Madden, University of Oxford, UK
Earth & Planetary Science	Professor James Holton, University of Washington
Mathematics	Professor Pierre Van Moerbeke, Department of Mathematics Cyclotron Research Center at Louvain-la-Neuve, Belgium Professor Cedric Villani, Ecole Normale Superieure De Lyon France
Mechanical Engineering	Professor Xanthippi Markenscoff, University of California San Diego
Molecular and Cell Biology	Professor Bengt Mannervik, Uppsala University, Sweden
Physics	Professor David Olive, University of Wales

Next Steps

Miller Fellow Jun Korenaga has been appointed Assistant Professor in the Department of Geology at Yale University beginning January 2003.

Miller Fellow Marius Crainic has been appointed a position as a KNAW Fellow and a member in the Mathematics Department at the University of Utrecht, The Netherlands beginning January 2003.

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Check our website for upcoming Deadlines

Miller Fellow Focus: Ben McCall

On the observational side, McCall and Geballe had a breakthrough at UKIRT by detecting H_3^+ in the well-studied diffuse cloud towards the bright star zeta Persei (which lies between the California Nebula and the Pleiades). This detection is particularly exciting because the ratio of electrons to hydrogen molecules (f) in this cloud has already been measured using ultraviolet satellite spectroscopy, and the size (L) is constrained by observations of other atoms and molecules.

Combining the results of the CRYRING experiment and this new observation, the three uncertain parameters k_e, f, and L are all pinned down. In effect, this means that the H_3^+ measurements can now be converted to measurements of the cosmic-ray flux (ζ), for which there are no other reliable measurements. Quite surprisingly, the inferred value of ζ is 40 times higher than the generally adopted value (which is the one that has been determined in dense clouds). If confirmed, these measurements suggest that a large flux of low energy cosmic rays pervades the galaxy, forming H_3^+ in diffuse clouds but unable to penetrate into dense clouds. Followup observations are planned at UKIRT and Keck Observatory.