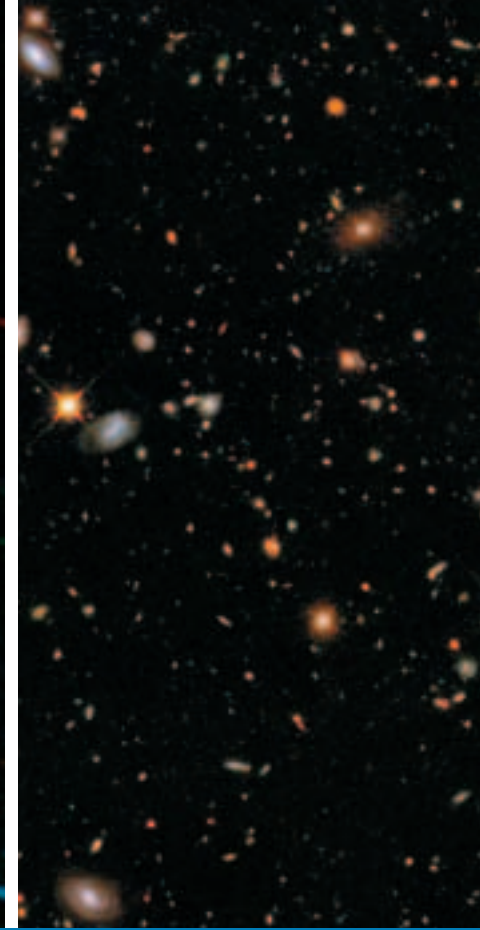
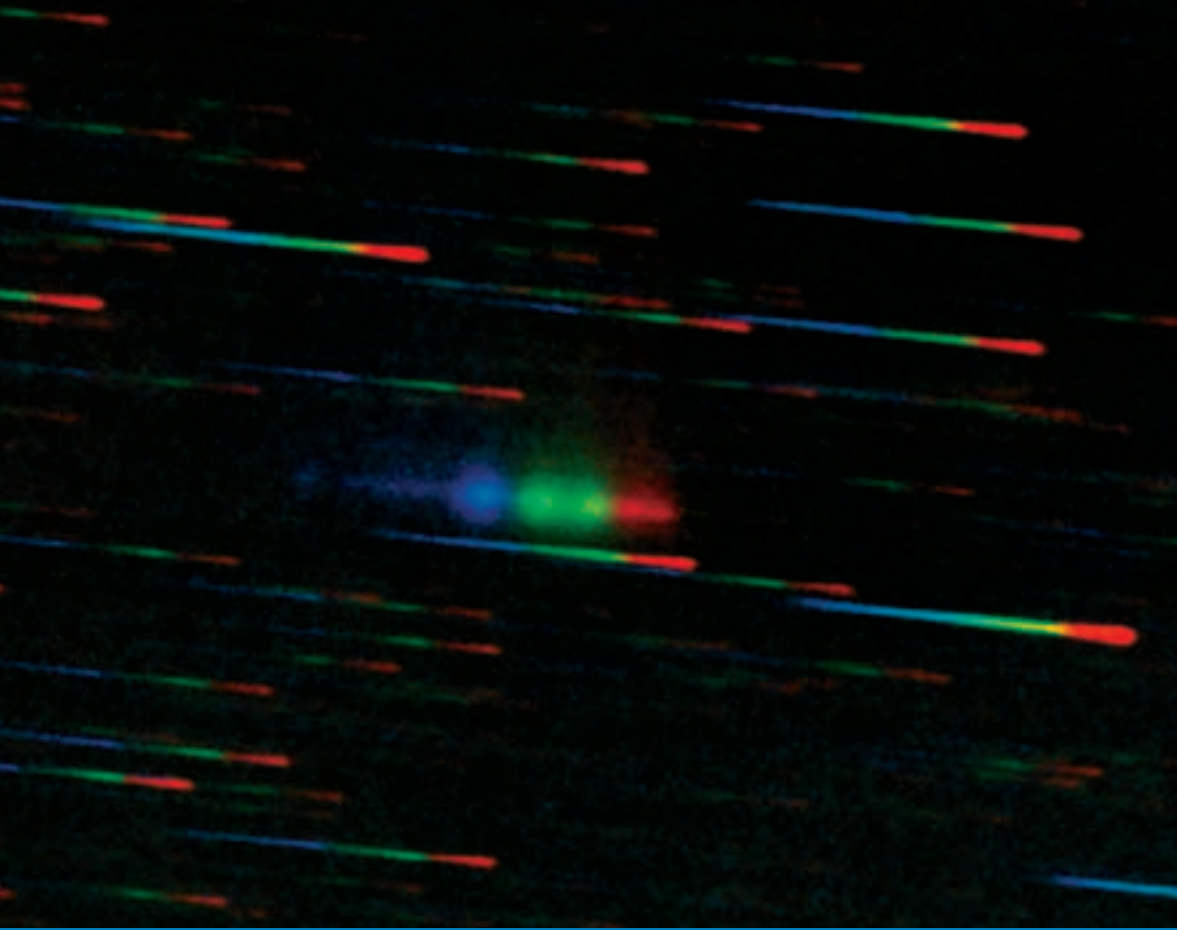


CHRIS SCHUR



Cosmic Code Breakers

By Daniel Wolf Savin,
Benjamin J. McCall,
and Kate Kirby

{ Not all professional astronomers use observatories to ply their trade. Some are hard at work in the laboratory, unraveling the mysteries of the universe. }



WHAT ARE INTERSTELLAR clouds made of? What are the properties of matter surrounding supermassive black holes? Why do ice-cold comets emit high-energy X-rays? The answers to these questions are encoded in the spectra from these objects. In fact, spectroscopy is the most powerful tool we have for exploring the universe beyond the solar system.

The laws of physics tell us that each atom or molecule emits or absorbs radiation at certain characteristic wavelengths. Astronomers use a spectrometer to spread the light from a celestial object into its component wavelengths, much as a prism turns sunlight into a rainbow of colors. The lines in the resulting spectrum can be thought of as a unique “fingerprint” that can be used to identify particular atoms or molecules.

Since Joseph Fraunhofer obtained the first spectrum of our Sun in 1814 (*S&T*: August 2004, page 44), astronomers have worked with laboratory scientists and theorists to decipher the information encoded in cosmic spectra. Their efforts have enabled countless breakthroughs in many fields,

including the discovery of helium, the understanding of which chemical elements were produced in the Big Bang, and the elucidation of the life cycles of stars.

Every cosmic spectrum contains a message. Reading this message requires an understanding of the underlying atomic, molecular, nuclear, and solid-state processes that generate the light. Laboratory astrophysics is the Rosetta Stone that enables astronomers to read spectra. This research includes experimental and theoretical work, each of which is necessary to benchmark the other. Theory can explore physical conditions too extreme to replicate in a laboratory, while experiments can measure things too complicated to calculate theoretically. Without this behind-the-scenes work, astronomers would have no way to interpret the spectra of stars and other objects in the universe.

Let’s look at a few examples of how interactions between observations, experiments, and calculations are enabling researchers to unravel some of the universe’s most perplexing mysteries.

Above: Much of what we know about the universe has been gleaned from spectra of astronomical objects, including stars (left), galaxies (center), and comets (right). But to identify features in the objective-prism spectrum of the star field (which includes a comet) shown at left, astronomers must compare their observations with lab spectra of the atoms and molecules thought to be responsible for these features. Without such detective work, the pattern of emission and absorption revealed by spreading starlight into its component colors would be indecipherable.

Diffuse Interstellar Bands

Stellar spectra contain many dark lines, mostly caused by atoms in the star's atmospheres that absorb light at specific wavelengths. In the early 1900s astronomers made a startling discovery: some of the absorption lines are caused by wisps of diffuse gas between us and the stars. These diffuse interstellar clouds are only about a billionth of a billionth as dense as Earth's atmosphere. But their enormous sizes imply that their total masses can reach that of 10,000 Suns.

Building on work by laboratory spectroscopists, astronomers identified some of these spectral lines as coming from atoms, such as sodium, potassium, and titanium, and small molecules, including CH, CH⁺, and CN. In recent years, scientists have detected larger molecules, such as C₃, H₃⁺, and HCO⁺. With such success, you might think that these clouds are well understood.

But they're not. Substantial numbers of absorption features in stellar spectra remain unidentified. Mary Lea Heger observed the first two of these in 1919 at Lick Observatory. They're broader than other lines, and they appear fuzzy or diffuse in photographic spectra, so they've come to be known as diffuse interstellar bands, or DIBs.

Subsequent observations have shown that hundreds of DIBs exist, and that they must be due to large (probably organic) molecules. But we have absolutely no idea what molecules these are! It is amazing that our ignorance about the DIBs has lasted so long, considering that most of the other questions astronomers were asking 80 years ago have long since been answered.

The solution to this mystery is conceptually simple: scientists guess a molecule that might be responsible for a DIB, obtain its laboratory absorption spectrum, and see if it matches the DIBs observed in stellar spectra. These guesses

are based on our limited knowledge of the chemical and physical conditions in diffuse interstellar clouds, as well as on any other information we can gather or calculate about the spectrum of a molecule. It's not easy to guess correctly: so far, no one has succeeded. And a correct guess requires that we recreate near-interstellar conditions in the laboratory.

One of the groups studying the spectra of potential DIB candidates is coauthor Benjamin McCall's at the University of Illinois. This team is in hot pursuit of the spectrum of the ionized soccer-ball-shaped molecule C₆₀⁺, a likely suspect for two DIBs seen at near-infrared wavelengths. To produce these ions, they heat neutral C₆₀ in solid form in an oven to 650°C (1,200°F). This vaporizes the C₆₀, generating a gas that expands through a tiny port into a vacuum chamber. The expansion causes the molecules to cool to -243°C, comparable to interstellar temperatures. As the gas expands, a high-voltage discharge (like a neon sign) ionizes the gas to produce C₆₀⁺.

McCall's group uses a sophisticated laser-based technique called cavity ringdown spectroscopy to detect absorption lines. Two highly reflective mirrors directed toward each other form a cavity that contains the potential DIB carrier, such as C₆₀⁺. Tunable laser light injected through the back of one of the mirrors bounces back and forth between them, effectively traveling several kilometers through the gas inside the cavity. As the researchers tune the laser wavelength, the decay rate of the light passing through the gas varies, revealing the absorption spectrum of the potential DIB carrier.

Laboratories around the world are pursuing experiments on potential interstellar molecules. But despite enormous efforts and a few false leads on the part of both laboratory and astronomical spectroscopists, so far, the quest to identify the molecules causing DIBs remains unfulfilled.

When a star field looks redder than it should, as this one does, astronomers know that there's dust and gas between us and the stars. Indeed, stellar spectra in fields like this display hundreds of absorption lines, some of which appear to be caused by interstellar clouds. Called diffuse interstellar bands (DIBs), these particular features remain unidentified nearly 80 years after their discovery. At the University of Illinois, researchers in coauthor McCall's lab (*inset, far right*) are studying the laboratory spectrum of C₆₀⁺, a possible carrier of some DIBs. The inset at near right shows what a DIB spectrum looks like without "contamination" from stellar or atmospheric absorption lines.

DIB
{diffuse interstellar bands}

BENJAMIN MCCALL / UNIV. OF ILLINOIS

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BENJAMIN MCCALL / UNIV. OF ILLINOIS



HARVARD-SMITHSONIAN CENTER FOR ASTROPHYSICS

Cometary X-Rays

The excitement of astronomy often comes from the discovery of unanticipated phenomena. For example, since the 1950s we have known that comets are lumps of ice and dust orbiting the Sun (*S&T*: February 2006, page 36). We see them because they reflect sunlight. Nobody expected anything so cold to emit high-energy X-rays. Yet that's exactly what Carey Lisse (Johns Hopkins University) and his coworkers discovered in 1996 when the Röntgen X-ray satellite (ROSAT) observed X-rays from Comet Hyakutake during its close approach to Earth. Astronomers have since observed X-rays from many other comets.

The source of the X-rays was originally a mystery. X-rays are usually absorbed by matter and are not easily scattered or reflected. The observed cometary X-ray emission was much stronger than could be explained by direct reflection of solar X-rays.

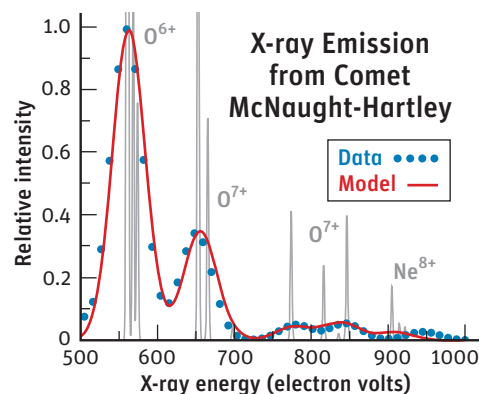
Astronomers knew that the solution to this mystery lay in the cometary X-ray spectra. But ROSAT's instruments had poor spectroscopic resolution. Using ROSAT data was like trying to identify a criminal from a blurry fingerprint.

In 1997 Tom Cravens (University of Kansas) proposed that the solar wind was the culprit. It consists of electrons, ionized hydrogen and helium, and trace amounts of other ionized elements such as carbon, nitrogen, and oxygen, all streaming out from the Sun. Cravens realized that these ions could capture an electron from neutral water or carbon dioxide molecules in a comet's coma. These electrons would be captured into orbits far from the atomic nucleus. As they decayed to smaller orbits, they would emit X-rays.

Soon afterward, Vasilii Kharchenko and Alex Dalgarno (Harvard-Smithsonian Center for Astrophysics) carried out some of the first theoretical calculations of the X-ray spectra resulting from solar-wind electron capture. They calculated what atomic orbits the electrons are captured into, how the electrons cascade from higher to lower orbits, and what wavelengths the emitted X-rays should have.

The 1999 launches of Chandra and XMM-Newton, along with archival data from the Extreme Ultraviolet Explorer, helped unravel the mystery. These satellites had spectrom-

X-ray {cometary X-rays}



SOURCE: V. KHARCHENKO & OTHERS / ASTROPHYSICAL JOURNAL

How can frozen comets like Hyakutake (*far left*) and McNaught-Hartley emit high-energy X-rays? By interacting with energetic solar-wind ions. Based on this mechanism, laboratory astrophysicists obtain promising agreement between a model spectrum and one recorded by the Chandra X-ray Observatory. *Inset*: Vasilii Kharchenko, Alex Dalgarno, and coauthor Kate Kirby (left to right) study astrophysics at the Harvard-Smithsonian Institute for Theoretical Atomic, Molecular and Optical Physics.

eters with resolution sufficient to unsmudge the spectral fingerprints. In combination with the theoretical models it was now clear that the X-rays were indeed coming from the solar-wind electron-capture process.

The criminal had been caught, but important differences remained between the observed and modeled cometary spectra. One explanation for these discrepancies might be incomplete models. If so, then such differences could be used as a guide to construct more sophisticated and potentially more accurate models. But another reason might also be errors in the underlying atomic data.

One of the groups of experimentalists who took up the challenge of benchmarking the theoretical atomic data is that of Ara Chutjian and his collaborators at Caltech's NASA/Jet Propulsion Laboratory in California. Their experiments begin with a microwave generator similar to those commonly used in household microwave ovens. They cook their ions to temperatures found in the solar atmosphere, thereby producing ions similar to those in the solar wind.

Next they accelerate these ions to the velocity of the solar wind, which ranges from 300 to 700 kilometers (200 to 400 miles) per second. The resulting beam then passes through a gas cell containing water or carbon dioxide (two of the main gases boiling off a comet). A germanium solid-state instrument detects X-rays created by the electron-capture process, yielding data that can test theory and enable astronomers to identify lines in the cometary X-ray spectra.

By combining theoretical calculations and laboratory data, scientists have built models that do a reasonably good job of predicting cometary X-ray spectra. Agreement is still not perfect, and several issues remain. But scientists are very excited over this newly discovered means of producing X-rays. For example, the solar-wind electron-capture mechanism also appears to be responsible for some of the X-ray emission seen from Mars, Jupiter, and Earth. The process is more widespread throughout the solar system than was first recognized. With future X-ray telescopes, improved calculations, and more laboratory measurements, it may even be possible that cometary X-ray spectra could be used to diagnose the properties of the solar wind.

Active Galactic Nuclei

Laboratory astrophysics can also help us understand the nature of black holes, among nature's most exotic objects. Black holes warp the fabric of space-time and generate copious X-rays. Particles are drawn into the black hole's gravitational whirlpool, emitting X-rays as they spiral down the drain (January issue, page 42). This outpouring of radiation blasts the surrounding material, stripping away electrons from atoms and creating a gas of free electrons and ions. Understanding a black hole's environment thus requires an accurate understanding of how electrons and ions interact.

Extremely massive black holes lurk in the cores of active galaxies, such as quasars and blazars (*S&T*: July 2006, page 40). The radiation emitted by these active galactic nuclei (AGNs) can be so copious and energetic that they sometimes outshine the hundreds of billions of stars in the host galaxy.

The Chandra and XMM-Newton X-ray observatories have given astronomers important insights into the extreme conditions near AGN central engines. For example, spectra from both satellites reveal mysterious structures in the outflowing winds surrounding the central black holes. But our ability to model the physical properties of these regions is hampered by uncertainties in our knowledge of the electron-ion collisions that produce the observed spectra.

Recent X-ray observations indicate that the iron in the

AGN winds is less ionized than predicted. Nature, of course, knows the correct ionization level of the gas. But sophisticated computer models are the only way we have to calculate the equilibrium between electron-ion recombination and ionization due to the X-rays from the AGN. This balance determines the average ionization level of the gas.

Hagai Netzer (Tel Aviv University, Israel) recently proposed that unreasonably low theoretical recombination rates for iron are responsible for the differences between the observations and models. If scientists change the models to reflect that, they might agree more closely with the observations.

Theory has provided most of the needed recombination rates. Yet more than 90 years after the discovery of quantum mechanics, atomic theorists still cannot reliably calculate many collision processes. This is a testament to the theoretical and computational complexity of modern physics, and it makes clear the importance of having reliable laboratory measurements with which to benchmark the theoretical calculations.

Using facilities such as the heavy-ion Test Storage Ring (TSR) at the Max Planck Institute for Nuclear Physics (MPI-K) in Heidelberg, Germany, laboratory astrophysicists can study here on Earth the same collisions that occur in AGNs. The TSR research is an international collaboration

AGN

{active galactic nuclei}

Supermassive black holes **{A}** lurk in the brilliant cores of active galaxies. Much of the high-energy emission from these active galactic nuclei (AGNs) is channeled into oppositely directed jets of radiation and particles that produce extremely complex X-ray spectra. An AGN is so luminous that it can outshine the hundreds of billions of stars in its host galaxy.

The Test Storage Ring **{B}** at the Max Planck Institute for Nuclear Physics in Heidelberg, Germany, provides an ideal arrangement for simulating atomic collisions in active galactic nuclei. To study low-energy electron-ion recombination, ions are injected into the ring at the lower right and are steered and focused clockwise along the 55-meter-long ring. The orange dipole magnets bend the beam, and the red quadrupole magnets focus it. The platform on the left side of the picture houses the electron beam, which merges with the ions.

This Chandra X-ray spectrum **{C}** of the active galaxy NGC 3783 is rich in absorption lines from ionized oxygen, neon, magnesium, and iron atoms. The observed absorption spectrum (in blue) closely follows the laboratory model (in red) except between 15 and 17 angstroms, where the model is still uncertain.



S&T: CASEY REED

MAX PLANCK INSTITUTE FOR NUCLEAR PHYSICS

involving the groups of Andreas Wolf (MPI-K), Alfred Müller (University of Giessen, Germany), and coauthor Daniel Wolf Savin (Columbia University).

The TSR experiment involves accelerating a beam of negatively charged iron ions and passing it through a thin foil. Collisions inside the foil rip electrons from the iron nuclei, creating a beam of positively charged iron ions. The more electrons that are stripped away, the more highly ionized the iron.

The beam is then injected into the TSR, which has a 55-meter (180-foot) circumference. The stored ions zip through the ring at 1% the speed of light. In one section, they merge with a beam of electrons and run together for about 1.5 meters. Over this length the beams mimic the electron-ion collisions that occur in AGNs.

Using the TSR facility, scientists are now measuring the crucial electron-ion recombination rates for iron ions. Recent work indicates that the published theoretical rates are indeed too low. Incorporating these new laboratory results into AGN spectral models will help astrophysicists better understand AGN winds and the properties of the matter surrounding the central black holes.

The Field's Future

Every generation sees major enhancements in the spatial

and spectral resolution of new telescopes and detectors. With these advances comes a parallel demand for more extensive and more precise understanding of the underlying processes that produce the observed spectra.

Laboratory astrophysics is an interdisciplinary field spanning traditional disciplines of physics, chemistry, and astronomy. It is the foundation for much of astronomical science. Unfortunately, NASA budget cuts have drastically reduced the available funding (*S&T*: June 2006, page 16), imperiling this cross-cutting, critically needed research.

In the future, many more cosmic mysteries will confront us, especially as we expand our view of the cosmos through new ground- and space-based observatories, all constructed at great expense. Only with a continued investment in laboratory astrophysics will astronomers be poised to unravel these mysteries and to extract the best scientific understanding from their observations. *

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