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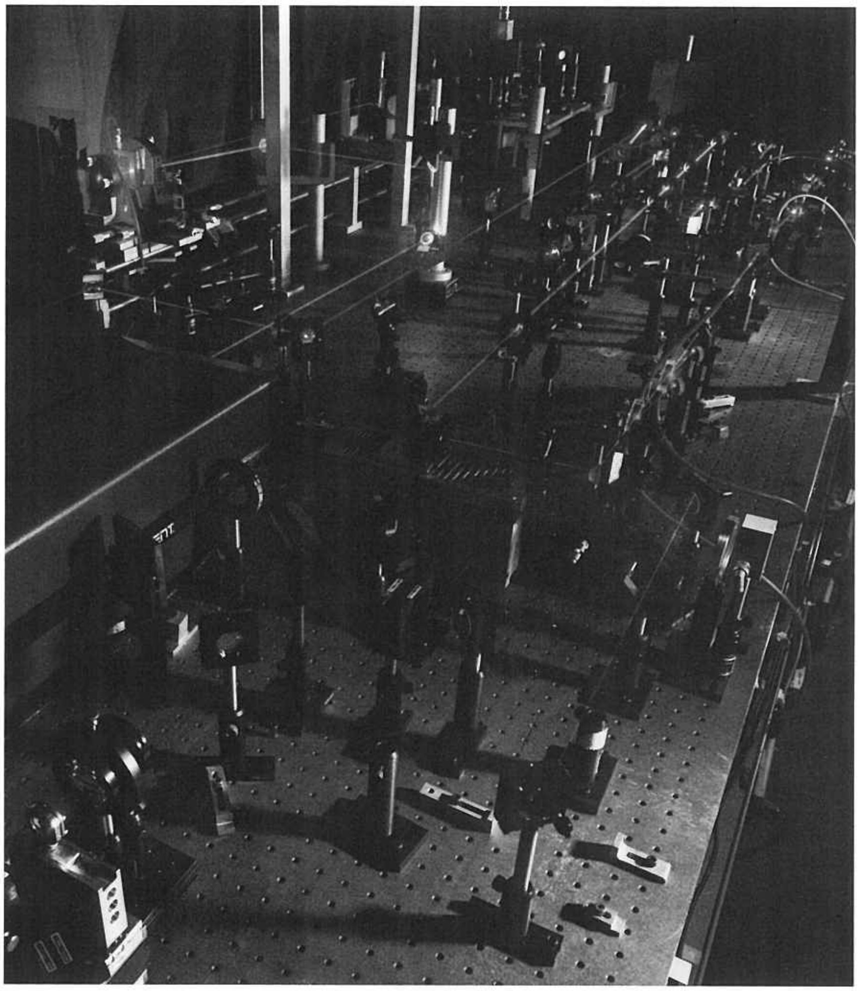

CN92-853

Ultrafast Infrared Spectrometer

The Ultrafast Infrared Spectrometer provides unique information on the ultrafast changes in molecular structure that occur during chemical processes. The instrument was developed to observe energy conversion and storage processes in proteins and in photochemical systems but is widely applicable to problems in chemistry, catalysis, bioscience, solar energy conversion, and the dynamics of materials.

William H. Woodruff, Isotope and Nuclear Chemistry Division; R. Brian Dyer, Kristen A. Peterson, and Page O. Stoutland, Chemical and Laser Sciences Division

At Los Alamos National Laboratory, we have developed the Ultrafast Infrared Spectrometer, which allows scientists to "see" the ultrafast changes taking place in molecules during chemical processes—changes that occur in less than a trillionth of a second. These changes, such as bond making and breaking, electron transfer, isomerization, and vibrational relaxation, reveal important information about mechanisms of chemical reactivity, materials dynamics, energy conversion and storage, catalysis, and chemical processes essential for life, such as photosynthesis and respiration.

By measuring on an ultrafast time scale the amount of infrared light absorbed by a sample, either at a single wavelength or over a spectrum, our Ultrafast Infrared Spectrometer provides scientists with direct, unique information about structural transformations that occur during chemical processes. Because the infrared spectra are sensitive to such properties as the strengths of interatomic bonds and the masses and locations of the bound atoms, this instrument enables us to take a series of closely timed "snapshots" that record changes in a sample's molecular structure.

No other spectroscopic method has both the speed and the sensitivity to structure that are required to follow ultrafast molecular changes. For example, commercial time-resolved Fourier transform infrared spectrometers have, at best, time resolution 10 million times longer than the resolution of our instrument. Likewise, transient electronic spectroscopy can be used to measure speeds of ultrafast reactions; however, the electronic spectra do not generally reveal the details of structural changes taking place in molecules during these reactions.

Our Ultrafast Infrared Spectrometer won a 1993 R&D 100 Award, an honor given annually by *R&D Magazine* to the one hundred most significant technical innovations of the year.

The Invention—Characteristics and Advantages

The Ultrafast Infrared Spectrometer uses a "pump-probe" approach, which involves generating two separate pulses of laser light, each a trillionth of a second long. The first of these pulses, the "pump," is of visible or ultraviolet light, which is absorbed by the sample, initiating the events to be measured. The second, the "probe" pulse of infrared light, provides the means for monitoring the changes induced by the pump. The spectrometer simultaneously measures the transmittance of the infrared probe through a sample that has been illuminated by the pump pulse and the transmittance through an "unpumped" reference sample, and it records the difference to provide information on the infrared absorbance. To obtain absorbance spectra, we record the absorbance changes at many different probe wavelengths and reconstruct the spectrum from the multiwavelength data.

Using the speed of light as a clock, our spectrometer can measure the speed of changes taking place during the pump-probe experiment. (Conventional electronics are not fast enough to track these ultrafast changes.) By varying the distance traveled by the pump pulse, and hence the time lag between the pump and the probe, we can measure absorbance versus time at a given infrared wavelength and thus measure the speed of specific structural changes.

Several design features make the Ultrafast Infrared Spectrometer unique. Its use of specific filters and refractive media allows us to select from a wide range of pump

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and probe wavelengths. Our ability to select virtually any wavelength in the visible and ultraviolet regions of the spectrum for the pump pulse means that we have essentially unlimited versatility as to which molecular systems can be studied with this instrument. Because we can tune the probe pulse throughout the infrared spectrum, we can follow structural changes in virtually any bonded structure or record infrared spectra over a broad wavelength range to maximize structural information.

In addition, by converting the probe pulse into a multiwavelength continuum, dispersing the pulse into its spectral components after it passes through the sample, and measuring the dispersed pulse using a detector with simultaneous multiwavelength capability, our spectrometer can record a substantial portion of the infrared spectrum while maintaining ultrafast time resolution.

Applications

The Ultrafast Infrared Spectrometer is a research tool for studying the basic steps in molecular dynamics. We have used the spectrometer to study energy conversion and storage processes in respiratory proteins and in photochemical systems; we are trying to identify the elementary physical or chemical steps and their accompanying structural transformations that occur when chemical or photochemical energy is processed in these systems.

Our first-generation Ultrafast Infrared Spectrometer will lead the way to further developments in instrumentation and basic science. This technique can be applied to many different areas of research, such as solving problems in chemistry, catalysis, bioscience, solar energy conversion, and materials science. ■

William Woodruff is a Laboratory Fellow in the Spectroscopy and Biochemistry Group of the Isotope and Nuclear Chemistry Division. He earned a Ph.D. in inorganic chemistry from Purdue University. He completed a postdoctoral fellowship at Princeton University and served on the faculty at Syracuse University and the University of Texas. He came to Los Alamos in 1984. His research interests are in inorganic photochemistry, transition-metal-containing biological systems, and chemical applications of lasers.

Brian Dyer is a staff member in the Photochemistry and Photophysics Group of the Chemical and Laser Sciences Division. He came to Los Alamos in 1985 as a postdoctoral fellow in the Spectroscopy and Biochemistry Group after earning a Ph.D. in chemistry from Duke University. His research interests include chemical applications of lasers and vibrational spectroscopy; bio-inorganic chemistry, photochemistry, and photophysics of metalloproteins and processes involving small-molecule binding and activation; and spectroscopy and dynamics of proteins.

Page Stoutland earned a Ph.D. in organometallic chemistry from the University of California at Berkeley. He completed a postdoctoral fellowship at Stanford University before coming to Los Alamos in 1989 as a postdoctoral staff member in the Spectroscopy and Biochemistry Group. He is currently a staff member in the Photochemistry and Photophysics Group. His research interests include ultrafast events in inorganic and organic chemistry and biophysical reactions.

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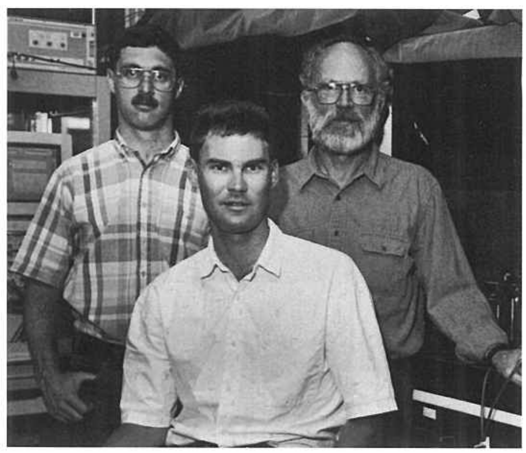

Three inventors of the Ultrafast Infrared Spectrometer are (from left) R. Brian Dyer, Page O. Stoutland, and William H. Woodruff. The fourth inventor is Kristen A. Peterson.

Kristen Peterson earned a Ph.D. in physical chemistry from Stanford University. Her research interests include ultrafast optical spectroscopies and other means for understanding intermolecular interactions, biophysics, and complex molecular systems. She came to Los Alamos in 1989 as a postdoctoral fellow with the Photochemistry and Photophysics Group. She left Los Alamos in 1992 for a postdoctoral fellowship at the Medical Free Electron Laser Center at Stanford University.

Work on the Ultrafast Infrared Spectrometer, which began in 1990, was funded by the National Institutes of Health and Los Alamos' Laboratory-Directed Research and Development Program.

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