

## Cover Story

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## CHEMISTRY HIGHLIGHTS 2002

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## PHYSICAL CHEMISTRY

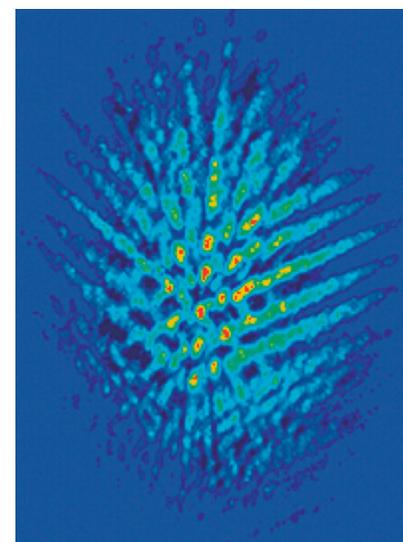
### STU BORMAN, C&EN WASHINGTON

In an eerie echo of the cold fusion controversy, a team led by Rusi P. Taleyarkhan of [Oak Ridge National Laboratory](#) reported that tritium and neutrons were produced in an acoustic cavitation experiment--by the fusion of deuterium nuclei inside collapsing bubbles formed in deuterated acetone bombarded with sound waves and neutrons [*Science*, **295**, 1868 (2002); *C&EN*, [March 11 page 11](#)]. But efforts to confirm this surprising result have been less than fully successful. And findings by [Kenneth S. Suslick](#) and a coworker at UIUC--that the maximum temperature generated in a bubble by sonochemical cavitation is far less than that needed for tabletop fusion--indirectly cast doubt on the ORNL findings [*Nature*, **418**, 394 (2002); *C&EN*, [July 29, page 11](#)]. In that study, the UIUC team made the first direct measurements of energy dissipation and reaction rates inside isolated bubbles that are generated by ultrasound.

In bimolecular nucleophilic substitution ( $S_N2$ ) reactions, it had been difficult to distinguish between steric effects and solvation effects on rate changes that occur when the carbon atom undergoing substitution is surrounded by different substituents. [John I. Brauman](#) of Stanford and coworkers used Fourier transform ion cyclotron resonance spectrometry to untangle those two key effects on reaction rate, and they found that solvation effects are much more influential than has generally been recognized [*Science*, **295**, 2245 (2002); *C&EN*, [March 25, page 10](#)].

After six years of supercomputer time, Iwao Ohmine, Masakazu Matsumoto, and Shinji Saito of Nagoya University simulated the freezing of unconfined water molecules to form ice crystals--a phenomenon that had eluded computer simulation for decades [*Nature*, **416**, 409 (2002); *C&EN*, [April 1, page 13](#)]. A better understanding of the kinetics and mechanism of ice formation could ensue.

[Stuart C. Althorpe](#) of the University of Durham, England; [Richard N. Zare](#) of Stanford; and coworkers obtained extensive experimental and theoretical support for the time-delayed appearance and predominantly forward trajectory of the HD product of the hydrogen-exchange reaction ( $H + D_2 \rightarrow HD + D$ ) [*Nature*, **416**, 67 (2002); *C&EN*, [April 1, page 62](#)]. The study aided fundamental understanding of the simplest chemical reaction.



**EXTREME** Diffraction pattern generated by the first spatially coherent laserlike extreme-UV beam, developed by Murnane and coworkers.  
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In a move toward achieving greater laser control of chemistry, Timothy S. Zwier and colleagues a

Purdue used a laser to isomerize N-acetyltryptophan methylamide [*Science*, **296**, 2369 (2002); *C&EN*, June 3, page 31]. They selectively excited single N–H stretch vibrational modes in the molecule. This propelled it into alternate conformations, with product distributions that depended on the conformation and mode excited.

The first spatially coherent laserlike beam in the extreme UV was developed by Margaret M. Murnane of the University of Colorado and the National Institute of Standards & Technology, Boulder, Colo., and coworkers [*Science*, **297**, 376 (2002); *C&EN*, July 22, page 10]. The tabletop system may be useful for imaging and generating holograms and diffraction patterns.

And using newly developed attosecond laser methods, Markus Drescher of the University of Bielefeld, Germany; Ferenc Krausz of Vienna University of Technology; and coworkers probed inner-shell electronic rearrangements in atoms in real time [*Nature*, **419**, 803 (2002); *C&EN*, Oct. 28, page 13]. "These inner-shell processes could not be probed at all in the time domain previously because neither the duration nor the photon energy of femtosecond laser pulses was satisfactory," Krausz tells *C&EN*.

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