and that the material in an electronic notebook may be inaccessible after the computer language changes. Some attendees suggested that if an electronic lab notebook is used, copies of it should be printed out periodically and signed by a witness.

David E. Wright, intellectual integrity officer at Michigan State University, East Lansing, pointed out that currently fewer than one in five graduate students has been trained to keep a rigorous lab notebook. Neither granting agencies nor graduate schools provide much guidance in this area, he said. "Writing the Laboratory Notebook," by Howard Kanare, published in 1985 by the American Chemical Society, is the only textbook on the subject, he said.

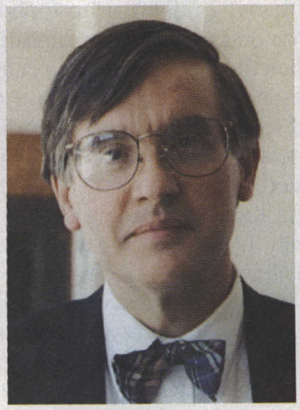
In recent years, when the need for careful record keeping has been greater than ever, Wright said, students have become sloppier about documenting their research. So now it is extremely important to provide training in record keeping, partly because research data have become more complex, he said. Data now may include X-ray film; photographs, negatives, and slides; printouts from computers; video and audio tapes; and computers and computer storage devices. "Many scientific instruments are coupled directly to computers, which digitize, analyze, and store data," he said.

Because interdisciplinary research collaborations are so common, Wright recommended that universities develop university-wide policies on research data management, rather than policies for each individual department. Such policies should include a definition of research data and guidance about how long they should be retained.

Defining exactly what research data are can be very difficult, especially when data can be created electronically, explained Walter J. Meyer, associate vice president for academic affairs at the University of Texas Medical Branch, Galveston. In his view, data should be defined very broadly. They should include "any lab work sheet, memoranda, notes and exact copies thereof, the results of original observations and activities, and studies that are necessary for the reconstruction and evaluation of the research report," he said. Data also should include output from the experiments, he explained, such as "synthetic compounds, organisms, cell lines, viruses, cell products, cloned DNA, DNA sequencing, mapping information, crystallography coordinates, plants, animals, and spectroscopic data of any kind."

Calculations performed on the data should be kept with the original data, so that the experiment can be pieced back together again, Meyer said. Data should not be recorded in hieroglyphics or in a foreign language that no one else at the university can read.

The University of Texas Medical Branch decided that data should be retained for five years after collection or five years after the date of its publication, Meyer said. It also decided that it owns all the data generated there, "although others might have access to them." The university "exercises its right to the data only under very special circumstances," such as when there are accusations of scientific misconduct, accusations of financial mismanagement, or concerns raised about intellectual property. Otherwise, the principal investigator is the custodian of the data. Faculty members at Meyer's institution have been asked not to sign contracts with industry that require permission before research is published.



Photos by Bette Hileman

(Clockwise from above) Oliver: meetings to review data; Davis: develop training handbooks; Staros: conventions of authorship

Bernard W. Janicki, director for research at the Dana-Farber Cancer Institute, Boston, explained how to prevent conflicts on research teams. Many conflicts can be avoided, he said, if "issues of leadership, authorship order, and intellectual property management" are "clarified and documented at the onset of the collaborative arrangement." In addition, oversight by the leaders of the institution and clearly defined policies and procedures are essential for successful management of collaborative research activities, he said. No honorary authorships should be allowed, he said.

According to David R. Challoner, vice president for health affairs at the University of Florida, Gainesville, lab directors will have much more success in maintaining high morale and high standards in the lab if students are mentored carefully. To be successful, he said, a mentor must be more than an adviser. The mentor should be "someone who takes a special interest in helping another develop into a successful professional," he said.

With graduate students, the primary obligation of their mentors is to further the students' education and to help them finish their degree programs in a timely fashion, Challoner said. Many graduate school faculty members around the country are significantly abusing the mentoring relationship, he observed. Some of them are more interested in the contributions the graduate students can make to their own research programs than in helping the students finish their degrees in a reasonable amount of time. It is especially important for mentors to help postdoctoral researchers focus their goals and find the next position.

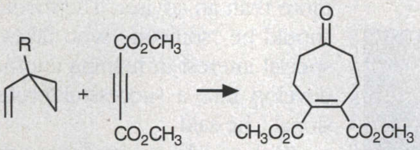
Few universities have formulated clear policies on research management, but meetings such as this one at the University of Arizona may stimulate them to develop such policies. ORI, part of the Department of Health & Human Services, plans to hold another conference on this topic in about two years.

The net result of efforts to manage research well, Pascal said, should be fewer allegations and actual instances of scientific misconduct.

Another result, Davis said, should be high-quality research and a high-quality education for students. "I'm a proponent of the student," he said. "Students are sometimes shortchanged." This has led to low graduation rates at some institutions, he noted. "A university's primary purpose is to teach, not to be a research institute."◀

Alkynes used to make seven-membered rings

A new class of transition-metal-catalyzed cycloadditions yields seven-membered rings from vinylcyclopropanes and alkynes, one of the most readily available classes of compounds [*J. Am. Chem. Soc.*, **120,** 10976 (1998)]. The reaction was developed by Stanford University chemistry professor Paul A. Wender and postdoctoral fellows Heiko Rieck and Masahiro Fuji.



They find that the reaction is remarkably general, with "electron-rich, electron-poor, conjugated, internal, and terminal alkynes, even acetylene itself," efficiently reacting under mild conditions. In the [5 + 2] cycloaddition, the five carbons of the vinylcyclopropane add across the two carbons of an alkyne, forming a seven-membered adduct that yields a cyclic ketone after acidic workup. For example, when the vinylcyclopropane shown here (R = *tert*-butyldimethylsilyloxy) is treated with dimethyl acetylenedicarboxylate in the presence of the dimer of rhodium dicarbonyl chloride at 40 °C for two hours, only one seven-membered cyclic ketone is formed in greater than 90% yield. Wender says the cycloadducts represent a new family of synthetic building blocks and could allow chemists to develop new ways to assemble complex molecules.◄

O_2-binding protein hemerythrin modeled

A key step toward a synthetic model of reversible O_2 binding in the protein hemerythrin has been taken by postdoctoral associate Tadashi J. Mizoguchi and chemistry professor Stephen J. Lippard of Massachusetts Institute of Technology [*J. Am. Chem. Soc.,* **120,** 11022 (1998)]. Hemerythrin is one of three known biological O_2-transport metalloproteins, the others being hemoglobin and hemocyanin. Synthetic small-molecule complexes that reproduce the active-site structures and ding properties of hemoglobin and hemocyanin have been made, but a synthetic model of hemerythrin has been elusive. In 1983, Lippard's group and Karl Wieghardt's group at Max Planck Institute of Radiation Chemistry, Mülheim, Germany, independently modeled an inactive diiron(III) form of hemerythrin. In 1985, Wieghardt also created a diiron(II) model, but it had no open site for O_2 binding. Mizoguchi and Lippard now have synthesized an inorganic diiron(II) complex that has an open O_2 binding site on only one of its two iron atoms, just as in deoxyhemerythrin, and that reacts with O_2 at low temperature. The oxygenated complex has spectroscopic properties closely matching those of oxyhemerythrin. The group hopes to eventually model both O_2 binding and release at room temperature with such a complex.◄

Combinatorial libraries: Two targets, one strategy

A single synthetic strategy may serve to synthesize multiple combinatorial libraries directed toward different therapeutic targets, according to medicinal chemists from Rhône-Poulenc Rorer, Collegeville, Pa. [*Angew. Chem. Int. Ed.,* **37,** 2848 (1998)]. Christopher J. Burns and coworkers note the similarity of the α-benzenesulfonaminohydroxamic acids that are matrix metalloproteinase (MMP) inhibitors and the phenylisoxazolecarbohydroxamic acids that are phosphodiesterase-4 (PDE4) inhibitors. MMP inhibitors show promise for treating cancer and arthritis. PDE4 inhibitors may alleviate arthritis and asthma. The investigators devised a convergent synthesis to produce two libraries of appropriately substituted hydroxamic acids that contain compounds active against each enzyme. This approach, they say, could help expedite the discovery of pharmaceutical lead compounds.◄

Polymer-nanotube composite shines

By dispersing small amounts of multiwalled carbon nanotubes in a conjugated light-emitting polymer, researchers have produced a composite that shows promise for optoelectronic and other applications [*Adv. Mater.,* **10,** 1091 (1998)]. Seamus A. Curran and Werner J. Blau of the physics department at Ireland's Trinity College Dublin and coworkers base their composite on poly(*m*-phenylenevinylene-*co*-2,5-dioctoxy-*p*-phenylenevinylene). The chains of this polymer tend to form coils that can wrap themselves around the nanotubes, yielding a stable composite with good nanotube-polymer interactions. The nanotubes were found to increase electrical conductivity of the polymer by up to eight orders of magnitude. And at low concentrations, the nanotubes do not appreciably diminish the polymer's luminescent properties. Furthermore, the nanotubes appear to act as nanometric heat sinks, preventing the buildup of heat (such as from laser illumination) that can degrade the polymer. Curran's team has used a thin film of the composite as the emissive layer in a light-emitting diode. Because the nanotubes boost the conductivity and mobility of charge carriers in the composite, it shines at lower current densities than does the pristine polymer, they report. Commercial development of the material is being pursued.◄

Mechano-catalytic water splitting claimed

Japanese researchers claim to have split water into hydrogen and oxygen by mechano-catalysis [*Chem. Commun.,* **1998,** 2185]. Earlier this year, the group at Tokyo Institute of Technology, led by chemistry professor Kazunari Domen, reported that copper(I) oxide can catalyze the splitting of water into H_2 and O_2 in visible light (C&EN, Feb. 16, page 26). But much to the team's surprise, subsequent experiments show that the gases continue to evolve in the dark for several hundred hours after the light is turned off. Similar results are observed with other binary oxides, such as NiO, Co_3O_4, and Fe_3O_4. The group hypothesizes that mechanical energy supplied by stirring is converted to chemical energy with the oxide functioning as a mediator or catalyst. "It is so simple and unexpected," Domen says. "By just rubbing a very common oxide in distilled water, you can get H_2 and O_2." However, Michael Grätzel, physical chemistry professor at Swiss Federal Institute of Technology, Lausanne, suggests that electrical charging of the powders by mechanical friction followed by local discharge may cause the water cleavage. Arthur J. Nozik, senior research fellow at the National Renewable Energy Laboratory in Golden, Colo., proposes other explanations—for example, that the oxides react with water in some kind of auto-redox process to produce H_2 and O_2.◄