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In This Issue



On the Surface

On the cover — an inhibitor (yellow) binds to the active site of the enzyme thermolysin in a computer simulation. The blue dots represent the enzyme's surface as seen by the solvent (water), and the yellow tetrahedron at center right is a zinc atom. Thermolvsin is a model for an enzyme that could be blocked by drugs to control hypertension, and the CLT inhibitor, as just such a drug (another view is on page 2), should bind tightly to the cleft in the enzyme's surface.

William Goddard and Barry Olafson predicted the optimum structure of this inhibitor theoretically; experiment has shown them correct. With high-speed computer techniques, theoretical chemists can calculate the forces on all the 3,500 atoms of a molecule like thermolysin in solution and predict optimum structures of molecules to bind to it. As Goddard explains in "Theoretical Chemistry Comes Alive," these new techniques have brought theory into its own in helping to understand how and why chemical processes work and in developing new materials with desired properties. He enthusiastically predicts a



revolution in what has been considered an empirical science.

His article. which begins on page 2, was adapted from Goddard's

Seminar Day talk last May, in which theoretical chemistry did indeed "come alive" for his alumni audience. Goddard is also a Caltech alumnus, having received his PhD in engineering science (with a minor in physics) in 1965. (His BS in engineering is from UCLA.) Although he did graduate work here with Pol Duwez in materials science, his interests were already turning to theory, and he became a research fellow in chemistry in 1964. Appointed assistant professor of theoretical chemistry in 1967, he became full professor in 1975.

During the 1970s Goddard's research began to concentrate on the properties of semiconductor and metal surfaces, and since 1978 he has been professor of chemistry and applied physics. Last year he was named to the first Charles and Mary Ferkel Chair in Chemistry and Applied Physics.

On Semantics

When Jean Weigle died in 1968, some of his friends established a memorial fund to bring lecturers of outstanding talent to Caltech's biology division. They hoped "to preserve the nearly extinct species of the scientist who is indifferent to the organizational aspects of science and is wholly devoted to the beauty of the scientific endeavor as a way of life." (E&S, January 1969)

The 1985 Jean Weigle Memorial Lecture was given last May by Gunther Stent. Before delivering his talk on "Meaning

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in Art and Science," Stent reminisced about the late 1940s at Caltech, when he was a research fellow, and Weigle, a physicistturned-biologist, had just arrived. Both worked with Max Delbrück, another physicistturned-biologist, in the "nascent discipline, which, a few years later, came to be styled 'molecular biology."



Before coming to Caltech in 1948 in the exciting years of Delbrück's Phage Group, Stent received his PhD in physical chemistry from the

University of Illinois (BS 1945). He left in 1950 for UC Berkeley. where he has been professor of molecular biology since 1959 and chairman of molecular biology and director of the virus laboratory since 1980.

Stent's article, which begins on page 9, was originally written for a Nobel Symposium, and it is reprinted here with permission of the Royal Swedish Academy of Sciences. It reflects his current thoughts in a debate about the relationship of art and science that has been running since his first article on the subject in 1972. Stent has also edited Delbrück's Mind From Matter? lectures, which Delbrück gave in the last years of his life, and which will appear in October as a book published by Blackwell Scientific Publications. Inc. E&S will print a chapter from the book in November.

PICTURE CREDITS: 10 — The Museum of Modern Art, New York; 12-13 - The Henry E. Huntington Library; 19-21 - Julie Scott; 24, 25, 27, 28 - Robert Paz; 29-30 - Richard Kee, Chris Tschoegl; 32 - F. Michelle Seyer

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Theoretical Chemistry Comes Alive

by William A. Goddard III



Top left. The optimized structure for CLT inhibitor (yellow) bound to the active site of the enzyme thermolysin. The tetrahedron represents zinc. The middle part of CLT Bottom left. Beta silicon nitride, a new ceramic, showing of the enzyme (the clamp). In the lower region the two parallel hexagons (corresponding to phenylananine residues) have a special stacking interaction (B. D. Olafson, W. A. Goddard).

Top right. The mayomycin molecule at the predicted bonding site of a CG tetramer of DNA (S. L. Mayo). is held in place by the hydrogen bonds to several residues the surface perpendicular to the c axis (M. M. Goodgame, W. A. Goddard).

Bottom right. Zeolite, A, showing the region accessible to solvent within one cavity (blue dots) (M. M. Goodgame, W. A. Goddard)

This article is dedicated to Linus Pauling, who blazed the trail for quantum mechanical contributions to the fundamentals of chemistry, and at 85 and professor emeritus of Caltech, is still active in unfolding the mysteries of nature.

HEMISTRY IS THE SCIENCE OF how electrons con--spire to bond atoms into molecules and solids and of how to rearrange these bonds to transform one combination of molecules into a specific new combination. Dealing as it does with the making and breaking of bonds, chemistry is the fundamental science underlying nearly all aspects of modern technology - from drug design, to plastics, to dyes, to catalysts, to high-temperature ceramics and metal alloys, to electronic materials for microelectronics. Unfortunately, despite the amazing progress in all these areas, we often do not really understand why current chemical processes work and consequently cannot predict how to develop new materials with specific properties. Rather, these areas of chemistry continue to develop empirically with clever experimentalists using analogy and intuition to try new procedures with varying conditions until they find a satisfactory solution. However, a revolution is brewing in which this situation should change dramatically, and I would like to provide here some of the flavor of these changes.

The underlying physics governing the motions of electrons in atoms and molecules is quantum mechanics, and when quantum mechanics was developed in the roaring twenties, there was hope that all of chemistry could soon be explained. Indeed, a great deal of progress did occur with theorists such as Linus Pauling at Caltech developing from quantum mechanics simple concepts of bonding that revolutionized the concepts of chemistry. There is, however, an enormous gap between the equations of quantum mechanics and the details of how to transform one chemical into another, and chemistry remained a highly empirical science. (In the same way, discovering that cells are composed of a bunch of chemicals did not explain biology.)

In recent years theorists have learned how to reformulate the basic quantum mechanics into a form where, with the aid of high-speed computers, accurate answers can be obtained for molecules of chemical, biological, and materials interest. This is most valuable, since the theorist can examine steps of reactions too ephemeral for experimental detection. Thus the theorist can examine the detailed trajectories of each atom during a reaction and can determine the properties of each reaction intermediate. However, this new-found ability to obtain such quantitative information will probably be less important than the ability of the theory to provide new *concepts* that collect together the quantitative results of theory and various experiments and that provide a *qualitative framework* useful for predicting how to modify the properties of a system.

By a conceptual framework I mean a simple picture that allows you to explain everything already known and allows you to predict how to change the system to do something new and neat. For example, one recent problem was to explain some puzzling tribological properties of the diamond surface. (Tribology is the science of friction and wear.)

The Diamond Surface

Diamonds are kind of expensive for bearings, but they do have very low friction (a coefficient of μ =0.1 up to 800°). Recently some researchers at a NASA lab found that when they heated diamond to about 850° C, the coefficient of friction all of a sudden increased dramatically (to $\mu=0.7$). At the same time the observed surface changed irreversibly so that it decomposed easily and led to other special properties. New electron levels appeared at the surface leading to color and a Schottky barrier (surface diode). But then when they exposed it to hydrogen, the friction came back down, the color disappeared, and the surface no longer decomposed so easily. If they heated it up again, all the problems returned as it got above about 850° C.

How can we explain this? Let's think a little bit more about the general properties of diamonds. Diamond is, of course, made of carbon atoms, and carbon has four valence electrons that can be used to make four



Figure 1: Carbon in diamond is bonded to four atoms arranged in a tetrahedron.



Figure 2: Each bond involves two electrons localized on two adjacent atoms but overlapping.

Contraction Contraction

Figure 3: Atoms at the surface can make three good bonds leaving one electron in a dangling bond orbital pointing into the vacuum.



Figure 4: Two pieces of unpolished diamond will have some surface dangling bond orbitals overlapping to bond the pieces together. This leads to high friction.



Figure 5: The surface dangling bond orbital of unpolished diamond leads to an energy in the energy gap (a). This leads to a Schottky barrier (surface diode) as in (b).

Figure 6: The top layer of unpolished diamond is unstable.

strong bonds. Inside the crystal the four atoms bonded to any carbon form a tetrahedron (figure 1). Each such bond involves two electrons, where one electron is localized more on one atom and the second electron more on the other atom, as indicated in figure 2. Carbons at the surface can't possibly make four bonds because one of these atoms would have to be sticking out in a vacuum. So at the surface you know there's going to be some kind of change in the properties of the system. The best a surface carbon can do (as in figure 3) is to make three good bonds with the fourth electron just hanging around doing nothing; it's called a *dangling bond* orbital.

What are the properties of such a system? The surface has these dangling bond orbitals sticking out into the vacuum just aching to make a bond with someone. Now let's put two such pieces of diamond together (as in figure 4) and slide them with respect to each other. The surfaces will not match perfectly, however; at the high points (asperities) orbitals of one surface will overlap the orbitals of the adjacent surface to form a covalent bond. As we try to slide the one piece of diamond, it is necessary to break these covalent bonds, leading to high friction. (We have to push hard to provide energy for stretching the bond as the surfaces slide along, but as a bond is formed, the excess energy gets converted into heat.) Indeed, if you cleave diamond in a vacuum and are quick about it, the pieces will adhere when you put them back together again. You can't wait too long because the surface is quite reactive and even in a good vacuum will quickly react with residual gas molecules until the dangling bond orbitals are mostly used up.

Having these dangling bond orbitals on the surface leads directly to other properties, making the surface very easy to oxidize and also giving it special semiconducting properties. Since each dangling bond orbital has one electron, it's very happy to accept a second one (getting spin-paired), leading to surface charges and diode properties (a Schottky barrier), as in figure 5. This dangling orbital



electron also makes it easy to absorb light, making the surface colored.

Even worse, the cleaved diamond has a tendency to decompose, forming graphitic regions. Why is that? The problem is that the surface carbon is only bonded to three things; but carbon bonded to three atoms likes to be planar (for example, CH, is planar). Thus each atom in the top row (say C_1 of figure 6) is yearning to get down to the next plane (to become planar). If the atom $(say C_{2})$ in the second row now moves up toward the surface row, the electron on the second-row atom (C_2) previously used to bond to the third-row atom (C_1) can now bond to the dangling bond orbital. Thus the process is to break the bond between the second and third row of atoms (a sigma bond) in order to make bonds between the second and first rows (pi bonds). Doing the same thing for adjacent surface atoms leads eventually to a layer of graphite on the surface. But now the third row of atoms looks just like the original first row. If you keep on doing this, the diamond decomposes - not too good if it's supposed to be for your girlfriend; it probably wouldn't even last the time of a California marriage.

How do we solve this problem? It was actually solved about a millenium ago by ancient diamond cutters, long before theoretical chemists came on the scene. What they did was to cleave the diamond in special kinds of oil. If you put a hydrogen atom (with its own electron) on each surface carbon, it bonds up with the dangling bond orbital to form a two-electron covalent bond. Now the surface carbon is perfectly happy being tetrahedral, and the surface is now perfectly stable. The surface won't react with oxygen, because there are no longer dangling bond orbitals for the oxygen molecule to bond to (singly occupied orbitals are needed to bond to one oxygen and thereby weaken the O-O bond before combustion can occur). Getting back to tribology, we see from figure 7 that there is also very little friction, because with hydrogen on the surface there are no dangling bond orbitals on adjacent surfaces to overlap. There is no chemical bonding between the surfaces — just very weak forces called Van der Waals interactions - and the surface now has the properties of a heavy hydrocarbon (wax). In addition, now that the surface orbitals are paired, they are too stable to play a role in the electronic properties (no room for an extra electron, too stable for

removal of an electron), so now the surface won't lead to color or to diode properties. In the last five years surface scientists have shown that polished diamond has a hydrogen atom at each surface carbon (figure 7) leading

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to all these neat properties while unpolished diamond (for example, diamond cleaved in a vacuum) has dangling bond orbitals and other crud on the surface.

Now that we understand all this we can go back and look at those experiments mentioned earlier. Polished diamond with a hydrogen on each surface carbon has low friction. At low temperatures it is way uphill for two hydrogen atoms to break their bonds to the surface and form an H₂ molecule. However at high temperatures the increased entropy of a free H₂ eventually favors desorption. This point occurs at about 850° C. Thus at 850° C the surface hydrogens come off as H₂, leaving dangling bond orbitals on the surface and all the properties of the unpolished diamond surface - high friction, color, and a tendency to decompose. Adding hydrogen again forms surface C-H bonds and all is hunky-dory (low friction, stable surfaces).

So now the question is, if we really understand things, how could we modify the system to get *different* properties? A good conceptual understanding allows us to make predictions on what we should do new to change the properties of the system. So let's say we want a diamond that would have low friction at 1,500° C (maybe diamond turbines for a new high-performance DeLorean). Is there some way to modify this system to make the surface more stable? We have to find something that will bond to each surface carbon, keeping it tetrahedral, but we want to make the bonds much stronger, so that the surface atoms won't leave the surface until higher temperature than hydrogen does. One possibility is to replace each hydrogen with a fluorine atom. The C-F bond is about 0.5 eV stronger than the C-H bond and, more importantly, the F_2 bond is far weaker (about 3eV) than the H₂ bond. Consequently we expect that the fluorinated diamond surface would be much more stable than the hydrogenated one. Simple estimates suggest that the fluorinated surface might be stable up to about 1,500° C. The fluorinated surface would also lead to low friction (like Teflon) and to other properties like those of polished diamond. (At Seminar Day I said that the experiment had not yet been done; since then I have learned of experiments at Rice University showing that the fluorinated surface retains low friction up to higher temperatures than the normal polished diamond.)

The important point here is to illustrate how a simple concept (about the nature of the surface bonding) can be used to predict a number of different properties of diamond (both polished and unpolished) and how this same idea can be used to design and predict the properties of modified systems. One concept can tie together experiments in completely different fields — from tribology to oxidation resistance, to the semiconducting properties, to the optical properties. They all tie back to this one concept of the tetrahedral bonding of carbon.

Catalysis

Another prime area of chemistry where theoretical chemists are getting into the act is making catalytic reactions selective. As an example, consider the molecule methanol (H_3 C-O-H). Adding oxygen to methanol can make carbon dioxide and water, but you can't sell them for very much. What you'd like to do sometimes is remove only two hydrogens and form formaldehyde, as in figure 8. But it's much easier to make car-



bon dioxide (making formaldehyde is about one-fourth as favorable). The challenge to the catalytic chemist is to design a system so that the reaction has a small hill to climb for going to the desired product and a much higher hill for going into the deeper valley of the detested reaction.

How does a theorist get ideas about what's going on in such a system? Let's consider molybdenum trioxide powder, which is

Figure 7: The polished diamond surface (terminated with H atoms) is hydrophobic and exhibits low friction.

Figure 8: Catalysis involves making the less favorable reaction go faster than the more favorable one by appropriately adjusting the barriers. MoO₃ does this to get nearly 100 percent H₂CO, but how does it work?



Figure 9: Two stable configurations for surface sites in MoO₃. Mo has six valence electrons and therefore makes six bonds. The left figure (mon-oxo) has one Mo=O double bond and four Mo-O single bonds (a total of six). The right figure (dual-oxo) has two Mo=O double bonds and two Mo=O double bonds for a total of six. In both cases the double bonds point into a vacuum so that no broken bonds are necessary.

Figure 11: We are halfway finished but can't finish the reaction if only one Mo center is involved.

Figure 12: If a second dualoxo site is close by, the second step of the reaction is favorable.

Figure 10: First steps: reacting H₂COH with the surface. The mon-oxo site is not favorable, but for the dual-oxo site the reaction to break the O-H bond is favorable because of the spectator oxo group. known to catalyze conversion of methanol selectively to the high-energy product (H_2CO) rather than the most stable product (CO_2). What we'd like to understand is what's happening on the surface. What are all the atoms doing, and why does it work that way?

Molybdenum has six valence electrons, and hence the most stable states of molybdenum have six bonds. This leads to two likely configurations on the surface, as indicated in figure 9. These species should be quite stable on the surface since there are no broken bonds.

What chemistry is expected for these surfaces? Janet Allison (PhD 1985) did the quantum mechanical calculations and found that the mon-oxo site (10a) is not very reactive. It's uphill to react with methanol. (Remember, our catalyst has to rip two hydrogen atoms off the methanol.) On the other hand, the reaction is favorable for the dual-oxo site (10b). The reason for such a dramatic difference has to do with the special properties that occur when an oxygen makes a double bond to a metal that already has another double bond. The second Mo-O double bond may not seem to be involved; however, this spectator oxo bond stabilizes the products resulting from reactions at the other double bond, thereby promoting the reaction. [The real story here is that Tony Rappé (PhD 1981), now professor at Colorado State, and I had discovered this spectator oxo stabilization effect while examining some reactions that occur in solution (homogeneous catalysis). and we guessed that such spectator oxo effects might play a role in reactions in molybdenum



crystals. We then looked into the chemistry of molybdates and got interested in the methanol-to-formaldehyde reaction. Of course, in the published research papers, we start off as if we had started off just to explain reactions on this neat surface.]

This is a start, but we've only done half the reaction; there is still another hydrogen to rip off, and the reaction won't be any good unless we can finish the job. Unfortunately with only one molybdenum center the second step of the reaction is unfavorable (figure 11). However, we find that the second step would be favorable if there were a second dioxo site close to the first one to pull off the second



hydrogen and make the final product (figure 12). Thus we concluded that a properly configured site with two dual-oxo units could be the catalytically active surface site for giving CH_3OH this one-two punch. The next question is whether the real surface can have such a configuration.



At this point in the research, Janet and I examined the bulk structure of molybdenum trioxide from x-ray structure studies and found that one surface, (010), of the crystal has exactly the configuration and the properties that we wanted (figure 13). Looking sideways at the surface there's a whole row of dual-oxo molvbdenum sites. This is the most stable surface plane (since no chemical bonds are broken in making the surface), and we found that this surface leads to a plausible catalytic cycle. At this point we ran across an experimental paper that had just come from France. These researchers had examined the catalytic reactions on itty-bitty molybdenum trioxide surfaces and found that one surface - precisely the (010) surface we had deduced - was responsible for the selective catalysis of H₃COH to H₂CO. We were really elated and rushed to finish the paper; we submitted



it a month later, saying that the French experiments proved our theory.

We then waited patiently for three months to get comments back from the referees. One referee said, Hey, this is really great work. It's good to see the theorists are finally doing something useful. Publish it. The other guy said, Well, it's interesting, but it can't be right. Some new experiments in an American industrial lab show that this surface is unreactive. We immediately located this new experimental paper, and it turned out that they hadn't actually done the chemistry. In a high vacuum system they had exposed the (010)surface of a single crystal of molybdenum trioxide to the CH₂COH, and since they didn't see any change in the spectroscopic properties of the surface, concluded that it's probably not reactive. But what they neglected to do is to expose the surface to oxygen. The French researchers had shown that if you don't have an atmosphere of oxygen on the (010) surface, you get no chemistry whatsoever. Presumably, without oxygen the catalyst loses some of its surface oxygen and hence loses the dioxo units required for the chemistry. So now my friends at this industrial lab are busy doing experiments adding oxygen to the surface. I should emphasize here that the theoretical results do not prove that the dual-oxo sites on the (010) surface do the chemistry. We have considered only the chemistry expected for these stable surface species. There could be an unstable species on this or other surfaces which is special to catalytic conditions and which would do the observed chemistry more rapidly. Now that there is a specific model (with a new principle — spectator oxo stabilization) for the surface configuration responsible for the catalysis, new special experiments will be designed to make specific tests of this model. As these tests proceed, the theorists will learn from the experiments and will examine various details more carefully. The result from

the theorists and experimentalists working together and separately will be a new level of understanding which will eventually lead to the knowledge needed to design new catalytic processes.

Simulation

The above examples focused on concepts about what the electrons are doing at surfaces and how to understand specific properties of various surface electronic states. There will be a flourishing of such theoretical activities in coming years; however, I believe an even more dramatic impact will come out of a related area of theory - computer simulation of materials processes. The idea here is to take the results of quantum chemical calculations on clusters of atoms (up to 10 or 20 atoms), as was used to get the numbers in the above sections, and to extract from these results an analytic description of energies and forces in terms of two-body, three-body, and four-body interactions. With such a description computer programs have been developed that allow the forces and dynamics of, say, 5,000 atoms representing the surface plus reacting atoms to be rapidly calculated on minicomputers (like the DEC VAX). With proper software the results of these calculations can be displayed in real time on a graphics system so that the scientist/engineer can actually "see" the reaction as it proceeds. With proper graphics equipment (such as the Evans and Sutherland PS 300), the user can interactively rotate and zoom the system to see the details in specific regions of the system and can pop the system into stereo to see the dynamics in 3-D. This overall process — Computer Aided Materials Simulation (CAMS) — will, I believe, have a significant impact upon the areas of drug design, chemistry (catalysis, synthesis, polymers), and materials research (ceramics, semiconductors, metallic allovs) even more dramatic than what CAD/CAM has done for the engineering design and processing communities.

At the moment biological systems are the only ones for which we have a good enough understanding of the forces so that we can reliably represent the quantum mechanics in terms of force field functions. The system illustrated on the cover (and at top left on page 2) is an enzyme, thermolysin, which is a model for an enzyme (angiotensin-converting enzyme) that you want to block in fighting hypertension. It's also resistant to high temperatures and so is a good model for research Figure 13: The (010) surface of MoO_3 . This surface shows the adjacent dual-oxo sites needed for the steps in 10 and 12. on commercial biocatalysis. Thermolysin has more than 3,000 atoms, and it's selective for breaking peptide bonds connecting hydrophobic (water-hating) amino acids.

Including a layer of water and some salt to mimic thermolysin in solution, postdoctoral fellow Barry Olafson and I used CAMS to calculate the forces on all 3.500 atoms as a function of time for simulations of the dynamics at various temperatures and to predict the optimum structure. In some of these systems experimental crystal structures were available for comparisons, and the excellent agreement confirmed the overall adequacy of the force fields. In the cover illustration the blue dots show the surface of the enzyme as seen by the solvent (water). The tetrahedron represents a zinc atom, and the entire cleft region represents the active site for this enzyme to bind to the substrate (the molecule it will cleave). A drug molecule to block the enzyme might be a molecule that would bind so strongly that it could not be displaced. Such an inhibitor (shown in yellow) was known from studies at Merck to be effective, but the structure was predicted theoretically without knowledge of the experimental structure. (Later comparison showed good agreement.)

The point is that theory is now in a position to give a credible prediction of structure even when there is no substantiating experimental evidence. Theory can also predict the interaction energies, which allows one to analyze why something (say, an inhibitor) works the way it does and then modify it on the computer to design an even better drug.

Probably the real payoff for theory in drug design over the next few years will be in understanding how various kinds of molecules bind to nucleic acids. This process plays a critical role in determining which genes are expressed and how fast, determining, for example, why the DNA in your earlobe makes earlobe cells and not brain cells. Olafson and I are now working on a regulatory protein binding to DNA but haven't yet optimized the structure. Using theory we're trying to calculate how the interactions work and predict how and where the protein wraps around the DNA. In a way we're in a race with experimentalists who are trying to cocrystallize this system so that they can do x-ray diffraction studies to get structure. (The experimentalists never believe that the theory can provide real predictions unless the theory was done before the experiment.)

As an alternative attack on this overall problem, grad student Steve Mayo has designed a molecule (top right on page 2 we call it mayomycin) to be selective for binding to sections of DNA that are rich in CG base pairs. The idea here is that if we can design a drug to recognize only a very specific sequence of base pairs, then we might be able to control the expression of a particular gene of a particular organism.

We're also working on understanding the forces for semiconductor surfaces so we can examine new synthetic techniques for making semiconductor devices (for example, the use of molecular beam epitaxy to make hetero-junctions and superlattices). We are also examining catalysis (such as in zeolites, bottom right on page 2) and ceramic surfaces to understand what happens when one ceramic rubs against another (tribology). The figure at bottom left on page 2, made by postdoctoral fellow Marv Goodgame, shows a surface for β -Si₃N₄, a new ceramic that is being developed for high-temperature gas turbines and adiabatic diesel engines.

A new project funded by the National Science Foundation will involve five Caltech faculty members interested in materials (Bill Johnson and Thad Vreeland from materials science. Marc Nicolet from applied physics, Tom Tombrello from physics, and myself from chemistry) who will carry out joint experimental and simulation studies to examine kinetic processes in materials synthesis. A unique aspect of this *Caltech Materials Center* (CMC) will be the integral use of simulation techniques in the various experimental programs. Because it is important for such a materials development program to have strong coupling with industrial research and development organizations, the group will probably involve a few industrial sponsors committed to a strong interaction with the CMC.

Various portions of the research reported were supported by the Department of Energy (Energy Conversion and Utilization Technology); the National Science Foundation (Division of Materials Research); the National Science Foundation (Chemistry Program); the Petroleum Research Fund of the American Chemical Society; the Office of Naval Research; and the Army Research Office. The software used for the biological simulation is BIOGRAF, written by Mayo, Olafson, and Goddard, and the hardware is an Evans and Sutherland PS-300/DEC VAX 11/780. □

Meaning in Art and Science

by Gunther S. Stent

In the fall of 1974, in the first issue of the new journal *Critical Inquiry*, there appeared a 50-page essay on the relationship of art and science by the University of Chicago musicologist Leonard B. Meyer. Meyer begins his essay by pointing out that for the past few decades that relationship has been the subject of confusing debate. Much of that confusion Mever attributes to doubtful analogies made by such people as "Gunther S. Stent, a molecular biologist [who recently] considered some of these matters . . . [and whose] discussion is representative of a viewpoint not infrequently espoused by scientists, and occasionally by artists and laymen as well. . . . Like a number of other writers, Stent contends that in essential ways science and art are comparable." Although Meyer expresses his sympathy for attempts to bring the so-called Two Cultures together, he doubts that their viable union can be achieved by ignoring or glossing over important differences. He says that he will argue "that Stent's union is a shotgun marriage, not one made in heaven, and that his attempt to wed different disciplinary species results not in fecund but barren misconceptions." What then is at the root of Stent's misguided attempt? It is, says Meyer, that "like many scientists (as well as a goodly number of artists and laymen), Stent fails even to recognize the existence of the humanist - that is, the theorist and critic of the arts." Meyer thus believes that a shotgun marriage between the Two Cultures is bound to fail because artist and scientist can only cohabit in a *ménage-à-trois*, with a humanist taken in as a housemate.

I felt honored that a brief popular article on art and science which I had published two years earlier in *Scientific American* (December 1972) had become the subject of a lengthy scholarly essay by a leading theorist of the arts. But I was taken aback by Meyer's critique, because I had believed all the while that in my article I presented merely a watered-down version of what I thought were Meyer's very own views; his book *Music, the Arts and Ideas* had actually been the main source of my ideas about the nature of art in the first place. I responded with a brief, aggressive rejection of Meyer's critique, and my response was, in turn, followed by a conciliatory rejoinder by Meyer and a final comment by the editor of *Critical Inquiry* expressing general agreement with both of us.

In the intervening years I have wondered why these debates about the relation of art and science are so confusing, why it seems self-evident that art and science are essentially similar and yet essentially different. Finally I came to realize that at the root of the difficulty is the unsolved, and possibly insoluble, deep problem of semantics, namely to say what it is that we are saying about a structure when we say that it has "meaning."

My article was inspired by my reading (and preparing a review) of the many reviews of James D. Watson's autobiography, The Double Helix (1968). Probably more than any other book, Watson's personal account of his and Francis Crick's discovery of the structure of DNA contributed to the latter-day demise of the traditional view that science is an autonomous exercise of pure reason carried out by disembodied, selfless spirits inexorably moving toward an objective knowledge of nature. The reviews of *The Double Helix*, almost all of them written by scientists, turned out to provide (mainly unwittingly) as much insight into the sociology of science and the moral psychology of contemporary scientists as does the book itself. Sir Peter Medawar was one of the few initial reviewers who recognized the considerable literary merits of Watson's book. He predicted that it would become a classic, not only in that it



Gunther Stent with a portrait of Max Delbrück painted in 1947 at Cold Spring Harbor by biochemist Efraim Racker.

will go on being read, but also in that it presents an object lesson on the nature of the creative process in science.

But the biochemist Erwin Chargaff, who himself has an important role in Watson's story, found as little merit in Watson's literary attainments as he had in Watson and Crick's discovery of the DNA structure in the first place. Not only did Chargaff not care for Watson's book, but he declared that scientific autobiography is a most awkward literary genre. The reason for this awkwardness is, according to Chargaff, that scientists "lead monotonous and uneventful lives. . . ." But why are the lives of scientists so monotonous and uneventful, in contrast to the exciting lives of, say, artists, who make much less trite biographical subjects? Because, according to Chargaff, there is a profound difference in the uniqueness of the creations of artists and scientists: "Timon of Athens could not have been written, Les Demoiselles d'Avignon could not have been painted, had Shakespeare and Picasso not existed. But of how many scientific achievements can this be claimed? One could almost say that, with very few exceptions, it is not the men that make science, it is science that makes the men. What A does today, B and C and D could surely do tomorrow."

Picasso's Les Demoiselles d'Avignon (1907). (The Museum of Modern Art, New York; acquired through the Lillie P. Bliss Bequest).



On reading this passage, I was surprised to find Chargaff embracing the "great man" view for the history of art, that is to say, regarding the development of art as wholly contingent on the appearance of a particular succession of unique geniuses, while at the same time viewing the development of science from the Hegelian or Marxist perspective of historical determinism, which sees history as shaped by immutable forces rather than by contingent human agency. Since I found it hard to believe that Chargaff would really hold such incoherent ideas. I suspected at first that he had made his point about the irreplaceability of Shakespeare and the replaceability of Dr. A only to downgrade the importance of Watson and Crick's discovery. But I soon discovered that my suspicion was quite mistaken. In the following months I asked many scientific friends and colleagues whether they too think that the achievements of art are unique whereas the achievements of science are inevitable, and hence commonplace. To my surprise, I found that most of my respondents agreed with Chargaff in believing that we would not have had Timon of Athens if Shakespeare had not existed, but if Watson and Crick had not existed, we would have had the DNA double helix anyway. Therefore, the deficiencies of the proposition of differential uniqueness of the creations of art and science do not seem to be as self-evident as I had thought at first. Accordingly, I wrote my little article to show why this proposition has little philosophical or historical merit.

Here we reach my first, albeit just sociological, disagreement with Meyer, because he claims that my view is not infrequently espoused by scientists. But since in his critique Meyer restates Chargaff's proposition as a self-evident truth, it would be *his* view, and not mine, which according to my experience is not infrequently espoused by scientists. Certainly all the scientists quoted by Meyer turn out to share his view, except for C. P. Snow and Thomas Kuhn as whose accomplice he regards me in the shotgun-marriage piot.

In order to examine the proposition of differential uniqueness of creation, I provided an explicit statement of what I understood to be the meaning of the terms "art" and "science." Both art and science, I wrote, are activities that endeavor to discover and communicate truths about the world, about the reality in which we live our lives. Thus art and science share the central features of

discovery and communication, and hence both involve the search for novelty and the encoding into a semantic medium the meaning of what has been discovered. Where art and science differ fundamentally is in the domain of reality to which the semantic contents of their works mainly pertain. The domain addressed by the artist is the inner. subjective reality of the emotions. Artistic communications therefore pertain mainly to relations between private phenomena of affective significance. The domain of the scientist, by contrast, is the outer, objective reality of physical phenomena. Scientific communications therefore pertain mainly to relations between public events.

This dichotomy of domains does not mean, however, that a work of art is wholly devoid of all outer meaning. For instance, a Canaletto painting communicates something about the public phenomenon that was Venice of the settecento. Nor does it mean that a work of science is wholly devoid of all inner meaning. For instance, Freud's The Interpretation of Dreams is addressed mainly to the private phenomena of the subconscious. Hence, despite this fundamental difference in their principal foci of interest, art and science actually form some kind of thematic continuum, and there seems to be little point in trying to draw a sharp line of demarcation between them. In any case, the transmission of information and the perception of meaning in that information constitutes the central content of both the arts and sciences. In other words, works of art and works of science are not merely there. They have a semantic content; they are meant to mean something. A creative act on the part of either an artist or a scientist would then be his formulation of a novel, meaningful communication about reality. Meyer refers to this understanding of the meaning of "art" and "science," of which as we shall see, he disapproves, as "Stent's definition." I was greatly surprised to find myself as the eponym of a mere paraphrase of explications that I had gleaned from the standard writings on this subject, above all from those of Susanne Langer and Meyer himself.

So I was now ready to ask whether it is reasonable to claim that only Shakespeare could have formulated the semantic structures represented by *Timon*, whereas people other than Watson and Crick might have made the communication represented by their paper, "A Structure for Deoxyribonu-

cleic Acid," published in Nature in April 1953. Here it is at once evident that the exact word sequence of Watson and Crick's paper would not have been written if the authors had not existed, no more than the exact word sequence of Timon would have been written without Shakespeare, at least not until the fabulous monkey typists complete their random work at the British Museum. Thus paper and play are both historically unique semantic structures. But in assessing the creative uniqueness of a linguistic structure we are not concerned with its exact word sequence; we are concerned with the uniqueness of its semantic content. And so I readily admitted that it was very likely that meanwhile, even without Watson and Crick, other people would have communicated a satisfactory molecular structure for DNA. Hence the semantic content of their paper would not be unique.

As for the semantic content of Shakespeare's play, however, I pointed out that the story of the trials and tribulations of its main character, Timon, not only *might* have been written without Shakespeare but in fact was written without him. Shakespeare merely reworked the story of Timon he had read in William Painter's collection of classic tales, The Palace of Pleasure, published 40 years earlier, and Painter in turn had used as his sources Plutarch and Lucian. But then the creative aspect of the play is not Timon's story; what counts is the novelty of the deep insights into human feelings that Shakespeare communicates in his play. He shows us here how a man may make his response to the injuries of life, how he may turn from lighthearted benevolence to passionate hatred toward his fellow men. Can we be sure that Timon is unique as regards the play's semantic essence? No, because who is to say that had Shakespeare not existed, no other dramatist would have communicated very similar insights? Another dramatist would surely have used an entirely different story to treat the same theme (as Shakespeare himself did in his much more successful King Lear), and he might have succeeded in pulling it off.

Hence we are finally reduced to asserting that *Timon* is uniquely Shakespeare's because no other dramatist, although he might have communicated to us more or less the same insights, would have done it in quite the same exquisite way as the Great Bard. But here we must not shortchange Watson and Crick by taking for granted that Drs. B, C, and D who

eventually would have found the structure of DNA would have found it in just the same way and would have published a paper that produced the same revolutionary effect on contemporary biology. On the basis of my personal acquaintance with the people engaged in trying to uncover the structure of DNA in the early 1950s, I expressed my belief that if Watson and Crick had not existed, the insights they provided in one single package would have come out much more gradually over a period of many months or years. Indeed, as Sir Peter Medawar found in his review of The Double Helix, the great thing about Watson and Crick's discovery was "its completeness, its air of finality." Medawar thought that "if Watson and Crick had been seen groping toward an answer, ... if the solution had come out piecemeal instead of in a blaze of understanding, then it would still have been a great episode in biological history." But it would not have been the dazzling achievement that it, in fact, was.

Why, then, is it that so many scientists seem to believe in both the uniqueness of artistic creation as well as in the commonplace, inevitable nature of scientific discoveries? One reason I put forward was that most scientists simply are not familiar with the working methods of artists. They tend to picture the artist's act of creation in the terms of Hollywood: Cornell Wilde, in the role of the one and only Frederic Chopin, is gazing fondly at Merle Oberon, as his muse and mistress George Sand, while he is sitting down at the Pleyel pianoforte and, one-two-three, he composes his Preludes. As scientists know full well, science is done differently: Dozens of stereotyped and ambitious researchers are slaving away in as many identical laboratories, all trying to make similar discoveries, some of them succeeding and some not. They know that the vast bulk of by no means negligible research papers are published by the unknown yeomanry of science, and not by its immortal geniuses.

Artists, we might note, tend to conceive of the scientific act of creation in equally unrealistic terms: Paul Muni, in the role of the one and only Louis Pasteur, is burning the midnight oil in his laboratory. He has the inspiration to take some bottles from the shelf, he mixes their contents and, Eureka, he has discovered the vaccine for rabies. Artists, in turn, know that art is done quite differently: Dozens of stereotyped and ambitious writers, painters, and composers are slaving



Title page and frontispiece of a 1734 edition.

away in as many identical garrets, all trying to produce similar works, all using more or less the same knowledge and techniques, some succeeding and some not. They know that the vast bulk of by no means negligible books, pictures, and tunes are produced by the unknown yeomanry of art, usually for mundane purposes, and not by its immortal geniuses.

A more serious obstacle is the apparently widespread confusion between works on the one hand and their contents on the other. A play or painting is a work of art, whereas a scientific theory or discovery is not a *work* of science but the *content* of a work such as a book, paper, letter, lecture, or conversation. Thus, as formulated, Chargaff's proposition of differential uniqueness is not even false; it is nonsensical, because it compares a *work* of art (*Timon*) with the *content* of a work of science (the DNA double helix).



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Not only Chargaff but even Meyer, a theorist of the arts, seems unable to keep in mind the difference between works and their contents. For he is going to "cut through [Stent's] Gordian argument with a sharp but simple distinction: Namely there is a profound and basic difference between scientific theories, which are *propositional*, and works of art, which are presentational" (emphasis in original). Meyer's antinomy is patently false, because all works, of science as well as of art, indeed all semantic structures, are "presentational" (in Meyer's sense being a concrete pattern that can be occasion for experiences that are found to be enjoyable, intriguing and moving). By contrast, the quality of being "propositional" (in the logico-philosophical sense of being a statement that affirms or denies something, so that it can be characterized as true or false) pertains not to works but to their contents. And here it is the case that

not every "presentational" structure necessarily has a propositional content. For instance, Meyer rightly points out that a natural phenomenon, such as a sunset or Mount Everest, is a presentational structure without propositional content. One of our principal agenda items will, therefore, have to be the question of whether the contents of works of art do or do not resemble the contents of works of science in being propositional. We will return to this central question later.

A second reason I advanced for the belief in the inevitability of scientific discoveries is the support which that belief appears to derive from the often-told tales of famous cases in the history of science where the same discovery was made independently two or more times by different people — for instance, the independent invention of the calculus by Leibniz and Newton, or the independent recognition of the role of natural selection in evolution by Wallace and Darwin. As the study of such "multiple discoveries" by Robert Merton has shown, however, on detailed examination they are rarely, if ever, identical. The reason they are said to be multiple is simply that in spite of their differences one can recognize a semantic overlap between them that is transformable into a congruent set of propositions.

As a third reason, I proposed that whereas the cumulative character of science is at once apparent to every scientist, the similarly cumulative character of art is not. For instance, it is obvious that no present-day working geneticist has any need to read the original papers of Mendel, because they have been completely superseded by the publications of the past century. Mendel's papers contain no useful information that cannot be better obtained from any modern textbook or the current literature. In contrast, the modern writer, composer, or painter still needs to read, listen, or look at the original works of Shakespeare, Bach, or Picasso, which, so it is thought, have not been superseded at all. In spite of the seeming truth of this proposition, it must be said that art is no less cumulative than science, in that artists no more work in a traditionless vacuum than do scientists. Artists also build on the work of their predecessors; they start with and later improve on the styles and insights that have been handed down to them from their teachers, just as do scientists. To stay with our main example, Shakespeare's *Timon* has its roots in the

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equipment, and to Dr. G. E. R. Deacon and the captain and officers of R.R.S. *Discovery II* for their pert in making the observations. ¹Youge, F. B. Gerard, H., and Jevons, W., 'Phil. Mag., **40**, 149 (1920).

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MOLECULAR STRUCTURE OF NUCLEIC ACIDS

A Structure for Deoxyribose Nucleic Acid

A Structure for Deoxyribose Nucleic Acid We wish to suggest a structure for the salt of deoxyribose nucleic acid (D.N.A.). This structure has novel features which are of considerable biological interest. A structure for nucleic acid has already been proposed by Fauling and Corey¹. They kindly made their manuscript available to us in advance of publication. Their model consists of three inter-twind chains, will the phosphares near the fibre axis, and the bases on the outside. In our opinion, this structure is unsatisfactory for two reasons : (1) We believe that the material which gives the X-ray diagrams is the salt, not the free acid. Without the acidic hydrogen atoms it is not clear what forces X-ray diagrams is the salt, not the free acid. Without the acidic hydrogen atoms it is not clear what forces would hold the structure together, especially as the negatively charged phosphates near the axis will repel each other. (2) Some of the van der Waals distances appear to be too small. Another three-chain structure has also been sug-gested by Fraser (in the press). In his model the phosphates are on the outside and the bases on the inside, linked together by hydrogen bonds. This structure as described is rather ill-fielded, and for this reason we shall not comment the reason we shall not comment

this reason we shall not comment on it. We wish to put forward a radioally different structure for the salt of deoxyribose nucleic acid. This structure has two helical chains each coiled round the same axis (see diagram). We have made the usual chemisal assumptions, namely, that oach chain consists of phrsphate di-ester groups joining \$-p-deoxy-ribofurances residues with 3'.5' linkages. The two chains (but not their bases) are related by a dyai perpendicular to the fibre axis. Both chains follow right-handed helices, but owing to handed helices, but owing to the dyad the sequences of the atoms in the two chains run in opposite directions. Each bain locally resembles Fur-

in opposite directions. Each chain loosely resembles Fur-berg's model No. 1; that is, the barse are on the inside of the helix and the phosphates on the outside. The configuration of the sugar and the atoms near it is close to Furberg's 'standard configuration', the sugar being roughly perpendi-cular to the attached base. There

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It has been found a generation of the amounts of advantmentation of the amounts of advantmentation of guantine to cytosine, are always very close to unity for deoxyribose nucleis easid. It is probably impossible to build this structure with a ribose sugar in place of the deoxyribose, as the extra oxygen atom would make too close a van der Waslis contact. The previously published X-ray data⁴⁴ on deoxyribose inside a contact. The previously published X-ray data⁴⁴ on deoxyribose mucleis acid are insufficient for a rigorous test of our structure. So far as we can tell, it is roughly compatible with the experimental data, but it must be regarded as unproved until it has been checked against more exact results. Some of these are given in the following communications. We were not avare of the details of the results presented there when we devised our structure, which rests mainly though not entirely on published experimental data and stereo-themosel arguments. mical arguments.

It has not escaped our notice that the specific It has not escaped our notice that the specific pairing we have postulated immediately suggests a possible copying mechanism for the genetic material. Full details of the structure, including the con-ditions assumed in building it, together with a set of co-ordinates for the atoms, will be published

elsewhere. We are much indebted to Dr. Jerry Donohue for constant advice and criticism, especially on inter-atomic distances. We have also been stimulated by a knowledge of the general nature of the unpublished experimental results and ideas of Dr. M. H. F. experimental results and ideas of Dr. Wilkins, Dr. R. E. Franklin and their co

Watson and Crick's famous publication of the discovery of the DNA double helix. Reprinted with permission from Nature.

is purely ic. The two

works of Aeschylus, Sophocles, and Euripides. It was those authors of Greek antiquity who discovered tragedy as a vehicle for communicating deep insights into feelings, and Shakespeare, drawing on many earlier sources, finally developed that Greek discovery to its ultimate height. To some limited extent, therefore, the plays of the Greek dramatists *have* been superseded by Shakespeare's. Why then, have Shakespeare's plays not been superseded by the work of later, lesser dramatists, say by Shaw's or Brecht's?

Here we do encounter an important difference between art and science, namely the feasibility of paraphrase. The semantic content of a work of art — a play, a cantata, or a painting — is critically dependent on the exact manner of its realization; that is, the greater an artistic work, the more likely it is that any omissions or changes from its origi-

nal structure detract from its full meaning. In other words, to paraphrase a great work of art — for instance, to condense Timon for the Reader's Digest - without loss of semantic content requires a genius equal to the genius of the original creator. Such a successful paraphrase would, in fact, constitute a great work of art in its own right. The semantic content of a great scientific paper, on the other hand, can later be paraphrased without serious loss by lesser scientists. Thus the simple statement "DNA is a doublestranded, self-complementary helix" does communicate the essence of Watson and Crick's great discovery. But it took the writing of King Lear to paraphrase (and improve on) Timon and indeed King Lear has superseded *Timon* in the Shakespearean dramatic repertoire.

The last reason I adduced for the widespread acceptance of the proposition that artistic creations are unique and scientific creations are not is the prevalence of an incoherent epistemological attitude toward the phenomena of the outer and the inner world. The outer world, which science tries to fathom, is often viewed from the standpoint of materialism, according to which phenomena and the relations between them have no objective existence independent of the human mind and this real world is as we see, hear, smell, and feel it. Hence the outer world and its scientific laws are simply there, and it is the job of the scientist to find them. At the same time, the inner world, which art tries to fathom, is often viewed from the standpoint of idealism, according to which phenomena and relations between them have no reality other than their invention by the human mind. Hence there is nothing to be found in the inner world, and artistic creations are cut simply from whole cloth. Here B or C or D could not possibly find tomorrow what A found today, because what A found today had never been there in the first place.

This incoherent epistemological attitude is also held by Meyer, who argues that only scientists discover truths; they do not create anything, except maybe intrinsically ephemeral theories. After all, "the structure of DNA was what it was before Watson and Crick formulated a theory of its structure." The reason for this is, according to Meyer, that "we assume evidently on good grounds, that while our theories explaining nature may change, the principles governing relationships

in the natural world are constant with respect to both time and place." Artists, by contrast, he says, do not discover anything; they create their works, which had no prior existence.

In the 1960s and 1970s, Immanuel Kant's definitive resolution of the age-old epistemological conflict of materialism versus idealism made its impact on the human sciences, under the general banner of structuralism. Structuralism emerged simultaneously, independently, and in different guises in several diverse fields of study, for example in psychology, linguistics, anthropology, and biology. Both materialism and idealism take it for granted that all the information gathered by our senses actually reaches our mind; materialism envisions that thanks to this sensory information reality is *mirrored* in the mind, whereas idealism envisions that thanks to this sensory information reality is invented by the mind. Structuralism, on the other hand, provided the insight that knowledge about the world of phenomena enters the mind not as raw data but in an already highly abstracted form, namely as structures. In the preconscious process of converting the primary sensory data step-by-step into structures, information is necessarily lost, because the creation of structures, or the recognition of patterns, is nothing else than the selective destruction of information. Thus, since the mind does not gain access to the full set of data about the world, it cannot mirror reality. Instead, for the mind reality is a set of structural transforms abstracted from the phenomenal world. Any set of primary data becomes meaningful only after a series of operations has so transformed it that it has become congruent with structure preexisting in the mind.

Thus neo-Kantian, structuralist metaphysics leads to the recognition that every creative act in art and science is both commonplace and unique. On the one hand, every creative act is commonplace, in the sense that there is an innate correspondence in the transformational operations that different persons perform on the same primary data from inner and outer worlds. On the other hand, every creative act is unique, in the sense that no two persons are quite the same and hence never perform exactly the same transformational operations on a given set of primary data. I therefore concluded my article by paraphrasing Orwell, saying that even though all creative acts in both art and science are both commonplace and unique,

some creations may nonetheless be more unique than others.

Taking Meyer's essay as a paradigmatic contribution to the debate concerning the relationship between science and art, we can see that the source of the confusion in that debate is not so much the invocation of doubtful analogies as the intractable nature of the underlying cognitive problems. To bring these problems into focus, let us first disperse the epistemological fog reflected in Meyer's pronouncement that the term "discovery" pertains only to science, whereas the term "creation" pertains only to the arts. As we already noted, a scientific theory is an abstraction made from what Meyer calls the "natural world," which presents our senses with a near infinitude of phenomena. Hence in their work scientists necessarily select only a small subset of these phenomena for their attention. Thus, contrary to the naive materialist outlook that Meyer brings to the discovery of the DNA double helix, the structure of the DNA molecule was not what it was before Watson and Crick formulated it, because there was, and still is, no such thing as the DNA molecule in the natural world. The DNA molecule is an abstraction created by century-long efforts of a succession of biochemists, all of whom selected for their attention certain ensembles of natural phenomena, according to an evolving set of transformational rules. In other words, the DNA double helix is as much a creation as it is a discovery, and the realm of existence of the double helical DNA molecule is the mind of scientists and the literature of science, and not the natural world (except in so far as that world includes also minds and books). Hence as applied to science, the distinction between discovery and creation is devoid of philosophical merit.

However, Meyer's central objection to what he calls "Stent's definition," which explicates art and science as activities that endeavor to discover and communicate truths about the world, lies in his claim that the concept of truth is simply not applicable to art. If this claim were valid, then the contents of works of art could not be propositional (inasmuch as they would not be statements that affirm or deny something that could be characterized as true or false), and hence artists could not be said to "discover" anything. Artists would merely create presentational structures without propositional content, just as God creates sunsets, no one of which has a content of which it can be said that it is true or false. All the same, Meyer admits that, unlike sunsets, "great works of art command our assent. Like validated theories, they seem self-evident and incontrovertible, meaningful and necessary, infallible and illuminating. There is, without doubt, an aura of 'truth' about them." But Meyer insists, as indicated by his putting the word in quotation marks, that in this connection "truth" is being used only in a metaphorical sense. Why? Because according to the naive materialist standpoint from which Meyer approaches this deep problem, a literally true scientific proposition states what is actually and objectively the case, that is, is directly observable in the real world. And since there are no imaginable observations that could test the validity of the *content* of a work of art, it could be said to be "true" only in a metaphorical but not in a literal sense.

Viewing our cognitive relation to the world from the standpoint of structuralism, however, leads to a different literal concept of truth. Inasmuch as reality, to which truth relates, is a set of structural transforms which each person abstracts from a world of things, things that are, as pointed out by Kant, in themselves intrinsically unknowable, the notion of truth has to be more relaxed. Namely, a scientific proposition is true (for me) insofar as it is in harmony with my internalized picture of the world (that is, my reality) and commands my assent. This literal meaning of truth is obviously not an objective one, but a subjective one. It leads to the concept of objective truth only as long as I am convinced that a proposition that is true for me would also command the assent of every other person qualified to make this judgement. Here the ideal of an absolutely objective truth is reached only if God also assents to the proposition. And so from the structuralist viewpoint the use of the term "truth" in connection with the content of a work of art is not metaphorical at all: It is the very same literal usage as that applied to the content of a work of science. It is exactly by their command of assent that we come to believe also in the truth of scientific propositions. In the 35 years that I have spent as a working scientist, I have personally validated (if indeed validation is at all possible), or even examined the published records of the validation by others, only a small fraction of the scientific propositions which I believe to be true. The remainder simply command my

assent, for the same reasons that Meyer cites as the basis of the aura of truth of great works of art.

Finally we come to the problem of the semantic content of the works of art and science. The semantic difficulties that seem to lie in the way of discussing "semantic content" are unwittingly highlighted by the editor of Critical Inquiry. In his summing up of our little wrangle, he expressed his belief that there can be meaningful works of art without semantic content. This belief is clearly paradoxical (or oxymoronic), since the adjective "semantic" means "having or related to meaning." Meyer, by contrast, can hardly deny that works of art have semantic content. In one of my favorite chapters of his Music, the Arts and Ideas he showed that the transmission of information by the artist and perception of the intended meaning of that information by an audience is the central feature of art, or rather of traditional art. By contrast, latter-day "experimental" or transcendental art, such as chance music and abstract expressionism, differs from its traditional forerunners precisely in that it has abandoned the semantic function. Works of transcendental art do resemble sunsets or mountains in that, just as those natural phenomena, they are merely there, without intended meaning, for the audience to make of them what it will. Transcendental art is, therefore, not only excluded from "Stent's definition" of art, but, thanks to Meyer's own analysis, provides an exception that proves the rule.

Let us now return to the question of whether, or in what sense, the semantic content of works of art could be propositional. Meyer proposes that a work of art is a "concrete exemplification of relationships," in other words, that although the work is concrete, its content is abstract, in the sense that the artist has created it in order to allow a percipient to recognize the exemplification of something more general than the work itself. But how does the percipient manage to understand the relationships that are being exemplified? According to Meyer, the percipient submits the work to a semantic analysis based on what Meyer refers to as "propositional habits." What then is the difference between the propositions of science and the propositional habits of art? Habits, unlike scientific theories, Meyer says, are not explicitly formulated. So it follows that the content of works of art is propositional after all

(in that a relationship being exemplified can be characterized as either true or false) but that, unlike the explicit propositions embodied in the text of a work of science, the propositions embodied in a work of art are merely implicit in its structure. This certainly is a profound and basic difference between art and science, but not one that will "cut through [Stent's] Gordian argument with a sharp but simple distinction." Instead, it points to the fact that it is their differential use of language which places an obstacle in the way of a felicitous union of the Two Cultures (rather than the failure to set up a ménage-à-trois with a humanist as housemate). The propositions of science are explicitly formulated, being stated in ordinary verbal discourse, the modality that the human brain has evolved to employ for explicit communication. The propositions of art, by contrast, are implicitly formulated, being embodied in tonal and visual structures, modalities for whose semantic processing the human brain employs means other than those it calls on for the processing of speech.

Armed with this insight, we can now reconsider the thematic continuum presented by art and science with regard to their principal foci of interest in inner and outer reality. To use a mathematical metaphor, this continuum is a scalar whose metric is the degree of concern with outer reality. Music, which appears to be the purest art form and has the least to say about outer reality, lies at one end of this continuum. Accordingly, music shows the least thematic overlap with science, which lies at the other end. The content of works of music is more purely affective than that of any other art form, because musical symbolism very rarely refers to any models of outer reality, to which it could never do justice anyway; the meaning of musical structures thus relates almost exclusively to inner models. Musical symbolism is able to dispense with outer models because, according to Susanne Langer, "the forms of human feelings are much more congruent with musical forms

than are the forms of spoken language; music can *reveal* the nature of feelings with a detail and truth that language cannot approach." Hence music conveys the unspeakable; it is incommensurable with language, and even with representational symbols, such as the images of painting and the gestures of the dance. So-called "program music," such as Respighi's *Pines of Rome*, which *does* refer to models of outer reality, appears to be another exception that proves the rule, in that program music is generally accorded rather low aesthetic merit.

Thus the position of an art form on this continuum — that is, its relative proximity to science and the extent to which it is addressed to outer reality — seems closely related to the degree to which its symbolism is embedded in language. The visual arts - painting and sculpture - are still relatively "pure" art forms, as is poetry which, although it does resort to language as its medium, uses words in a quasi-musical form. But literature and drama, with their mainly linguistic symbolism and their close thematic ties to outer reality, but still addressing the inner reality of feelings, seem to lie halfway between music and science. Science is, of course, wholly dependent on language as its semantic modality, bearing in mind that mathematical notation has to be regarded as merely a time- and effort-saving shorthand mode of expressing complex logical relations between ordinary words.

All the same, the semantic transactions of art still pose a most difficult problem. What is the meaning of the propositions which are implicitly formulated in works of art? To what do the relationships exemplified by works of art actually refer? What are they about? Evidently the difficulty of answering these questions increases as we progress from science toward music in the thematic continuum. At the musical end of the continuum, where symbolism is incommensurable with language, these questions cannot be answered (verbally) at all. For instance, according to a



legend quoted by Meyer, Beethoven, when asked what the *Moonlight* Sonata means what it is *about* — went to the piano and played it for a second time. Meyer finds Beethoven's answer not only appropriate but compelling. But Meyer thinks that if a physicist were asked what the law of gravity is about and answered by letting some object fall to the ground, our inference would be that the physicist is disingenuously witty that he had not responded properly.

I agree that Beethoven's response seems more reasonable than that of the uncooperative physicist, but not for the reason given by Meyer, namely that the *Moonlight* Sonata is not about the world and does not refer to something. Rather, Beethoven's response is reasonable because he was asked a question for which there is no adequate verbal reply, whereas the physicist's response is unreasonable because he could have said something. This then is the paradox: Logic demands that since the *Moonlight* Sonata, exemplifying a relationship, has some meaningful content ---as opposed to a sunset, which has not — it must refer to something, must be about something. Yet we cannot say what that something is. In thus being generally speechless regarding the meaning of music, we resemble the split-brain patients studied by Roger Sperry, who can recognize familiar objects seen in the left half of their visual field but are unable to identify these objects verbally.

As we move away from music toward science in the thematic continuum, through the visual arts to literature and drama, verbal explanations of the meaning of art works, though still formidably difficult, become at least possible. Indeed it is the very task to which hermeneutics is dedicated, the discipline originally concerned with the interpretation of sacred and profane texts but which has been extended more recently to making explicit also the implicit meanings that are hidden in a broad range of semantic structures. There would be massive unemployment among contemporary hermeneuticians if Meyer's assertion that the contents of works of art do not refer to anything and are not about the world were actually true. Suppose, to stay with our original example, having just seen a performance of *Timon*, we asked a Shakespearean scholar what does the play mean — what is it *about* — and he simply took us back to the theater to make us see Timon for a second time. Would we not consider his response as disingenuously witty and as nearly improper as that of the physicist? That is not to say that if the scholar did give us his verbal interpretation of Timon, it would fully capture the semantic essence of the play. As we already noted, because of the difficulty of paraphrase, our scholar would have to be a genius equal to the Bard to accomplish that task. Nevertheless, depending on his hermeneutic skills, he could go some considerable distance toward giving us an idea what the play's deep meaning, and not just its plot, is about. What would be most likely missing from the scholar's verbal interpretation of *Timon* is precisely that part of the play's meaningful content which is not embedded denotatively in the text and which arises from it connotatively, thanks to the contextual situation created by Shakespeare. The obstacles in the way of foreign-language translation of verbal works of art would seem to reflect that same difficulty of paraphrase, as expressed in such homely saws as "tradutore, traditore" and "poetry is what is untranslatable in literature." Yet the fact that a poem cannot be rendered full justice in translation does not show that it is not about the world, that it does not refer to anything.

So we have traveled a long way from Chargaff's reflections on the triteness of scientific autobiography to the bottomless depths of epistemology and cognitive philosophy. As for marriages made in heaven, that of the Two Cultures would not be the first in which the spouses turn out to have some difficulties in talking to each other. So maybe it would be a good idea after all to keep a hermeneutic humanist as an interpreter in the Arts and Sciences household. \Box





Superstrings

YEAR AGO John Schwarz and Michael A Green announced a discovery that pointed the way toward tying up a lot of loose ends in physics. With a mathematical breakthrough in their superstring theory, they suddenly found themselves with a very promising candidate for a unified field theory describing all four known fundamental forces of nature — electromagnetism, the weak and strong forces, and gravity. The search for a unified field theory has been the most compelling problem in modern physics, whose solution was Einstein's dream; it has eluded physicists ever since. Although electromagnetism and the weak force have been established as being related to each other, and progress has been made toward linking up the strong force, until a decade ago the inclusion of gravity appeared to most theoretical physicists

a problem best avoided. Since then the search for a unified field theory has been an active subject of research, with today's theoretical physicists seeking a quantum mechanical field theory that would, at last, embed Einstein's general theory of relativity comfortably in quantum mechanics.

Not everyone has been looking for the solution in superstrings, a word coined by Schwarz. In fact, before August 1984 Schwarz, then senior research associate, and Green, visiting associate at Caltech (from Queen Mary College, University of London), may have been the only two people in the world working on superstring theory. Now hundreds have jumped on the bandwagon. Although not directly involved in the work, Murray Gell-Mann, Nobel laureate and the Robert Andrews Millikan Professor of Theoretical Physics, has been providing encouragement along the way and considers the recent work of extraordinary importance. "If it's not *the* answer, it's an important step in moving toward the answer," he says. "If superstring theory works, it will prove to be the key to early cosmology as well as particle physics."

In superstring theory all elementary particles are, instead of points as previously assumed, strings, albeit very short ones $(10^{-33} \text{ cm}, - \text{ a Planck length})$, that exist in 10-dimensional space-time. They're not just mathematical fictions, insists Schwarz, but really do exist as one-dimensional curves with zero thickness. But they're so small that for most practical purposes they are well approximated by points. The string-like structure becomes important only at extremely high energies (or very small distances) and could be directly observed, says Schwarz, only in experiments at 10^{19} GeV. Current accelerators are capable of only 10^3 GeV.

Such a bizarre picture (although Schwarz maintains that it's really quite conservative) didn't suddenly appear out of nowhere last year. The basic idea of strings, including some mathematical machinery for them, has been around since the late 1960s, when it was proposed as a theory of hadrons — the numerous different subnuclear particles including the neutron and proton, which are held together by the strong force. But there were a few problems with the original string theory of hadrons. For one thing, it contained tachyons, massless particles that travel faster than the speed of light, whose existence was essentially impossible. And it did not contain any fermions. Fermions are particles that obey the Pauli exclusion principle, that is, no two of them can simultaneously occupy the same quantum state. The basic fermions are the leptons (which include the electron, the muon, the tau, and their neutrinos) and



the quarks — building blocks of the hadrons. Besides the serious drawback of missing most of the particles, the theory also required a rather intimidating 26 dimensions of spacetime.

Fifteen years ago at Princeton, Schwarz and André Neveu, with a contribution from Pierre Ramond (who later also came to Caltech), set out to get rid of these difficulties. They came up with a version of the theory that incorporated fermions and that led to the elimination of the troublesome tachyons after the simple modification of consistently omitting certain parts of the theory. The number of dimensions of space-time was now 10 instead of 26. But although this new string theory was, according to Gell-Mann, "a beautifully consistent theory" and "very exciting," quantum chromodynamics emerged at about the same time (partly the result of Gell-Mann's own work and that of Harald Fritzsch, who was then also at Caltech) and was recognized as the correct theory of hadrons and the strong force. String theory was superseded as a theory of hadrons, and its popularity waned.

But Schwarz stuck with string theory anyway, convinced that, in Gell-Mann's words, "somehow, sometime, somewhere, it would still be useful." Schwarz came to Caltech at Gell-Mann's invitation in 1972, and in 1974 he and Joël Scherk hit on the idea that the key particle — of mass 0 and spin 2 — which had been so troublesome for the hadron interpretation, might actually be a graviton, the hypothetical particle that carries the force of gravity. What was impossible for a theory of hadrons and the strong force was "just what one wants for a graviton," says Schwarz. (A graviton will not be observed directly in the near future because its interactions are so weak, but it definitely does exist, Schwarz says.) And Einstein's theory of gravitation appeared as an approximation to the theory.

With the revival of the string idea in a new context, their whole perspective changed. They abandoned the attempt to make it fit hadrons and began to consider string theory as a possible quantum theory of gravity and all other phenomena as well. From this perspective the previously troublesome components of string theory settled quite neatly into place. Scherk and Schwarz reduced the hypothesized size of strings 20 orders of magnitude — from the size of the nucleus to 10³³ cm. They published papers in 1974 and 1975 reformulating Schwarz and Neveu's original string theory as a quantum theory of gravity. With the simple modification mentioned above, the reformulated string theory possessed supersymmetry and had supergravity (Einstein's theory of gravitation combined with supersymmetry) as an approximation.

A kind of supersymmetry arose out of Schwarz, Neveu, and Ramond's first string theory in 1971, when it was still being applied to hadrons. The more commonly discussed kind of supersymmetry was introduced for point particles at about the same time by a Russian group and later independently by Wess and Zumino in Europe. It involves a mathematical transformation that interchanges fermions and bosons (including the so-called gauge particles — photons, gluons, and gravitons, which shuttle between particles and transmit forces), so that each fermion has a boson partner and vice versa. These hypothesized particles have some fanciful names (Schwarz claims no responsibility for them); for example, the boson partners of quarks and leptons are squarks and sleptons, and the fermion partner of the photon is the photino. Observation of these predicted particles, which would confirm supersymmetry, may be possible with some of the powerful new colliders now on the drawing boards, or even with existing ones, Schwarz believes. The search has already begun.

One of the stumbling blocks of a quantum theory of gravity in which gravitons and other elementary particles are described as points is the occurrence of infinities. Supersymmetry turns out to play a crucial role in canceling out certain infinities. Calculations in quantum mechanical theories require contributions from all particles, the bosons in certain examples giving positive contributions and the fermions negative ones. When they are kept separate, you get the infinities that you don't want, but in superstring theory the fermion and boson contributions are combined. canceling each other out and producing finite results. This also happens to some extent in supergravity, although it is a point-particle theory, but not to an extent sufficient for meaningful finite results, according to Schwarz. In the late 1970s supergravity was itself a hot candidate for a unified field theory — so hot that Scherk and Schwarz's 1974 paper caused little stir. Very little was published on strings until Schwarz and Michael Green's first joint paper in 1981.

Green got involved with strings on meeting Schwarz at CERN, the particle physics



laboratory in Geneva, in 1979, and thus began a fruitful collaboration that has continued during several months of each subsequent year, on one side of the ocean or the other. Since supergravity had captured the attention of most others, the two were left in peace. "It was nice, really," says Green. "We could work on a topic and be sure that no one else had already done it." And their results were interesting to enough people (Gell-Mann and Edward Witten of Princeton, in particular), that at least "no one treated us as if we were crazy."

The most popular version of supergravity postulates 11 dimensions of space-time, which Green says is impossible, since the correct theory must be chiral, that is, left-right asymmetric, or mirror asymmetric, as are the laws of physics. He believes that chiral theories can exist only in an even number of space-time dimensions, such as the 10 dimensions of superstring theory, which Schwarz had already suggested in 1972. And where are the other six, apart from the three of space and one of time that we know? Presumably they're too small to be observed and are described as curled up, collapsed, or compacted into a sort of six-dimensional ball. While the nine spatial dimensions could have been equivalent in the first moments of the Big Bang, symmetry could break in the rapidly cooling and expanding universe, leaving three dimensions very large and six very small.

Although chirality is an essential feature of Schwarz and Green's theory, chiral fermions create what was thought to be an inescapable problem of anomalies (inconsistencies introduced by quantum effects). It was considered such a generic problem in higher dimension theories that theoretical physicists were stymied by it until the summer of 1984, when Green and Schwarz showed that anomalies could cancel in superstring theories.

Their calculations showed that there were no anomalies for superstring theory in the case of two specific symmetry groups — the breakthough that suddenly attracted so much attention. In particle physics symmetry groups, of which there are an infinite number of possibilities, are used to define transformations that relate particles to one another and thereby relate the properties of those particles. Quantum field theories that describe the fundamental forces of nature other than gravitation (electromagnetism and the weak and strong forces) use specific symmetry groups to describe the interactions and the quanta that carry them. These established and accepted theories have not used theoretical criteria to select symmetry groups but have picked them because they are the groups that fit the experimental facts. For example, the electromagnetic force is characterized by a group of transformations called U(1). A symmetry group labeled SU(3) describes the strong force of quantum chromodynamics, and SU(2) the weak force. Glashow, Weinberg and Salam received the Nobel Prize in 1979 for mixing the SU(2) and U(1) symmetry groups (the electroweak forces). The theory that encompasses all three symmetry groups (SU(3) \times $SU(2) \times U(1)$ is called the Standard Model, and it describes all the known forces and particles - except gravity.

Ideally, however, the symmetry group should be uniquely determined by the theory itself without having to "dial knobs" in the equations, as Schwarz puts it. Schwarz and Green found, not by dialing any knobs but by using superstring theory, that mathematical consistency (that is, elimination of the anomalies) made two particular symmetry groups pop out — groups designated SO(32) and $E_s \times E_s$. These are both very large symmetry groups (496 generators) easily able to encompass all known elementary particle symmetries. Schwarz and Green came up with a superstring theory with the SO(32) symmetry group that was free of anomalies and infinities, and just a few months later a group of researchers from Princeton, taking off from Schwarz and Green's work, presented a superstring theory for $E_8 \times E_8$. This particular symmetry group is especially exciting because it readily breaks down to the Standard Model. E_s had long been a favorite of Gell-Mann (and others), who had been hoping someone would find a string theory for it. Suddenly a

unified field theory looked to be within reach.

For Gell-Mann, one of the important answers superstring theory offers is to the question of the confusing and continuing proliferation of elementary particles. Why are there so many? Superstring theory suggests that there are actually an infinite number of particles, with only some of them lying in the low-mass states, that is, relatively low; in many cases the low-mass states are still high-mass states as far as experimental physicists are concerned. "But these infinitely many particles all obey a single very beautiful master equation," says Gell- Mann. He describes the theory as that of a field taken as a function of a one-dimensional path or string (which corresponds to an infinite number of functions of a point) in spacetime. Just as the strings of a musical instrument can yield an infinite number of harmonics, so the theory's strings can vibrate in an infinite number of modes.

The second E_s of the symmetry group brings with it a bizarre phenomenon of much interest to astrophysicists - shadow matter, that is, a whole other corresponding (although not exactly corresponding) type of matter that interacts with the matter we observe only through interactions of gravitational strength - that is, very weakly except in large aggregates. On the basis of observable behavior of galaxies, astrophysicists believe there must be a great deal of unseen "dark" matter exerting gravitational force - matter whose existence would determine whether the universe will forever expand or whether it will eventually collapse on itself. It is intriguing to consider that the E_a shadow matter, hidden from our perception, may provide the answer.

The potential of superstring theory is exciting, and, according to Green, "it may soon be able to explain a great deal of experimental information." This potential for explaining observed phenomena has put a lot of physicists in gear, notably the group at Princeton working with Witten. Mathematicians are getting involved too, in particular attempting to describe the geometry of the six curled-up dimensions. One likely possibility is that they form what is called a Calabi-Yau space, which is a type of six-dimensional space of great importance in pure mathematics.

"We've formulated the basic equations," says Schwarz, who is now professor of physics. "Now all we have to do is solve them." $\Box - JD$

Research in Progress

Under the direction of Fredrick H. Shair, professor of chemical engineering, and with the financial support of many corporations and individuals, the Summer Undergraduate Research Fellowship (SURF) program is providing stipends for 126 students this summer. This month's Research in Progress profiles four of these SURF projects.



California's First Barbecue?

Somewhere NEAR BARSTOW some 200,000 years ago a group of hominids may have dug a pit, surrounded it with stones, and set a campfire. Senior Janet Boley, working with Joseph Kirschvink, assistant professor of geobiology, is trying to determine whether an ancient ring of stones, looking for all the world like a carefully prepared hearth, actually housed a roaring fire. She's doing this by searching for the magnetic traces that would have been impressed on the stones by the fire's heat. Since most archaeologists believe that humans first came to North America between 12,000 and 25,000 years ago, Boley's results, if positive, would be revolutionary, pushing this date back by a full order of magnitude.

Several of these stone circles were discovered 50 feet under the surface of



Janet Boley points to a core hole she drilled in one of the putative ancient hearth-stones. She'll slice the core itself like a salami and will measure the magnetic moments of the resulting discs.

an alluvial fan - a cone-shaped deposit of sediment that forms at the mouth of a stream. Percolating ground water left a crust of caliche (calcium carbonate) on each buried stone, and this caliche has been dated by radiometric uranium/thorium methods to be at least 200,000 years old. Archaeologists have found thousands of possible human artifacts near the rings, most of which are apparently the remnants of stone tools. The majority of archaeologists would argue, however, that both the putative tools and the stone circles could have been formed by natural processes.

Boley's investigations of the magnetism of the stones may go a long way towards resolving this dispute. You can think of the stones as containing millions of magnetic crystals, each acting as a tiny compass, pointing in the direction that the earth's magnetic field pointed when the stone originally cooled from the molten state. When the postulated early human (who may actually have been a *Homo erectus*, the predecessor of *Homo sapiens*) gathered the stones and arranged them around the circle, the magnetic "moments" of each of the stones would have ended up pointing in a different random direction.

But the magnetic moments can be reset if their temperature is raised beyond the mineral's "Curie point." A roaring fire would have done just that, but only to the parts of the stones that got hottest, the parts facing the inside of the circle. And the magnetic moments of all the inside faces of the stones would have been reset to point in the same direction: the direction of the earth's magnetic field when the fire burned.

To test whether this actually hap-

pened, Boley drills cylindrical cores from each of the stones, carefully preserving the original orientation so that the core will go as directly as possible from the stone's inside to its outside face. She then slices these cores like a salami, ending up with discs that are the diameter of a quarter and a quarter-inch thick. Using a magnetometer, she measures the magnetic moments of each of the discs. She expects to see the direction of the magnetic moments gradually changing as she goes from discs that had been near the inside of the ring to those that had been near its outside. And when she correlates the magnetic moments of all the discs from all the cores taken from all the stones, she will see if the magnetic moments of the inside discs point in the direction of the earth's magnetic field, while the magnetic moments of the outer discs point in different directions from stone to stone. And, since different minerals within the stones have different Curie points, careful study may actually tell her not only whether a fire burned within the circle, but even just how hot that fire was.

Workers at the original site, along with JPL's Alan Gillespie, recently performed an important control experiment. They dug a pit, arranged locally collected stones in a circle around it, filled the pit with indigenous sagebrush, and lit a seven-hour bonfire, taking careful temperature measurements along the way. The glowing coals measured 700° C, and the stones measured 291° C on the inside, 90° C on the outside, and 200° C on the bottom. Boley is performing the same measurements on the control stones as on the others.

At this writing, measurements on only one core of one old stone have been completed. The results from this core are negative; there was no change in magnetic moment from one end of the core to the other. But Boley believes that the core may not have gone from the hot end to the cold end. and she's drilling another core from this stone oriented in another way. She's continuing with her measurements of cores from the other stones as well — both the actual ones and the controls — and she hopes to answer one of the most important questions in North American archaeology by the end of the summer. \Box -RF

Power of a Tourney

Most RESEARCH in mathematics relates to nothing in everyday experience and can't be described in ordinary language. But senior Art Duval is working on a project that is understandable to those unschooled in higher mathematics and may well have practical application too. He's working on the problem of ranking teams that have played an incomplete tournament.

There's no problem in ranking teams that have played a complete tournament, which is defined as one in which every team plays every other team exactly once. In that case, the highest ranking team is the one that wins the most games. But when every team doesn't play every other team, two problems arise in determining a ranking. One is the problem of cycles, in which team A beats team B, team B beats team C, and team C beats team A. The other problem is the problem of unbalanced schedules. Suppose there are 10 teams and half are tough opponents and half are easy opponents. Suppose further that team A plays four games against the easy teams, beating them all, while team B plays four games agains the tough teams, winning two and losing two. Because the schedules of A and B are unbalanced, it's difficult to compare their abilities.

There are some established methods for ranking teams in an incomplete tournament. These methods assume that each team has a certain amount of ability, which can be represented by a single real number. Given the results of an incomplete tournament, these methods attempt to determine how the unplayed games would most likely have come out. Duval, however, was bothered by the assumption that ability can be represented by a single real number and he decided to assume that a team's ability is indexed by two real numbers, representing, say, the separate abilities of the offense and the

defense. Having made this assumption, Duval's first task was to determine how the two components could interact. "If one team's numbers are 3 and 7 and the other team's are 5 and 5, which one is better? Well, if you just add them up, for instance, then you don't really have two numbers at all. A lot of other methods come to the same thing. So I spent some time trying to find an interaction that didn't collapse into the one-dimensional case."

The method he came up with involves taking the difference between the first components of the two teams and adding that to a constant times the difference between the second components raised to some power. Duval then ran extensive simulations



where the computer randomly generated pairs of abilities for 25 teams and played the teams against each other. He was trying to determine the best values for the constant and the power term, values that would maximize the number of cycles in the tournament. This would give him something to work with in the next stage, in which he would try to modify the established methods to determine the dual abilities of teams in an incomplete tournament. Determining the proper constants, however, quickly turned into a problem in statistics, a problem that Duval did not feel ready to tackle just then, so he set it aside and began working on the problem of avoiding unbalanced schedules.

"If everyone plays the same number of games and if you distribute them properly, then no one should have too unbalanced a schedule. Obviously, you can't say you've got a method that definitely will get it because no matter how you do it, you can define the rankings in such a way that someone's playing all the best teams. But you can minimize the probability of that. Imagine spreading all the teams out on a table like a bunch of marbles. You wouldn't want to just play everyone within a small distance of yourself because it would be difficult to rank yourself against ones in the far corner." Duval has just finished a course in graph theory where he came upon something that struck him as applying to this problem - a type of graph called a "strongly regular graph." Says Duval, "A graph is just a bunch a vertices (which you can think of as teams) connected by a bunch of edges (which you can think of as games)." Duval is currently analyzing strongly regular graphs in this light.

Duval's project falls under the branch of mathematics called combinatorics. His faculty sponsor, Richard M. Wilson, professor of mathematics, defines combinatorics as, "that branch of mathematics that deals with arrangements of finite sets of objects." But he qualifies that statement in the peculiar manner mathematicians use when trying to express in ordinary English their ineffable interests: "That definition is not precise; in fact, it's meaningless, but at least it's true."

Will Duval's work have practical

application? At first glance the National Football League with its 28 teams, each with a schedule of 16 games, seems like a perfect example of an incomplete tournament. "But they're not really after finding the best team," says Duval. "They're after selling lots of tickets." If the NFL could rank the teams after the regular season, there'd be no reason to go into playoffs. "As far as scheduling goes, there they also have different priorities. They're more interested in establishing rivalries than in making balanced schedules." But if the NFL isn't interested, other organizations may be. Food companies that conduct taste comparisons could use the methods Duval is developing to minimize the number of comparisons that they need to make to arrive at a valid ranking. Practical application, however, is not one of Duval's priorities. "Even if no application is found for 50 years, I think the math in it has turned out to be very interesting." $\Box - RF$



Dancing Sands

BENEATH THE SUB-BASEMENT of the Kellogg Radiation Laboratory, in a room shrouded in black plastic sheets, sophomore Minh Tran shoots BBs from an air gun into a BB-filled box in an attempt to simulate the movements of sand in the wind. These experiments, which Tran conducts under the supervision of Peter Haff, senior research associate in physics, should lead to a better understanding of wind erosion and sand and dust storms and may help explain the origin of sand ripples — a beautiful and universal, yet still poorly understood, natural phenomenon.

Wind-blown sand moves primarily by "saltating," a word that comes from the Latin *saltare*, which means "to jump." A grain of sand in the air is pushed forward, parallel to the ground, by the force of the wind, and it's pulled downward by the force of gravity. It hits the ground at an oblique angle and imparts its force to other sand grains, which jump off the ground, and are accelerated by the wind, eventually to strike still other sand grains a bit further on.

In fact, it is saltation that provides a rigorous definition for the word "sand." Sand particles, with typical diameters ranging from 0.15 to 0.3 mm, are just the right size to undergo saltation. Larger particles (pebbles) are too large to be bounced up and accelerated by the wind and are left behind as sand masses move. Smaller particles (dust) enter suspension in the air and can be blown many miles from their points of origin. Haff refers to the wind as "a giant winnowing machine" that separates sand from pebbles and dust.

With Tran's help, Haff is investigating three interconnected aspects of saltation. The first of these is a description of the aerodynamic forces acting on a sand grain. These forces, combined with gravity, determine the



To simulate sand blowing in the wind, Minh Tran fires BBs from an air gun into a BBfilled box, photographing the impact using two strobes. In the top photo a "sand grain" (coming from the right) blasts a number of others into the air.



grain's trajectory. The second aspect involves the feedback of the grains on the wind. As wind speed increases, it imparts more momentum to each sand grain, which in turn splashes up more grains at each impact. But additional airborne grains suck energy and momentum from the wind, damping it somewhat. In order to determine the extent of this damping, Haff needs to know the trajectory of the grains. But in order to describe the trajectory of the grains, Haff needs to know wind velocity. It's possible that this seemingly circular problem can be resolved by employing iterative calculations.

Tran is working on the third aspect of saltation, which involves describing the "splash function." He's trying to determine the distribution of splashed particles — how many are splashed up, how high they go, and what angles they go in — as a function of the energy and the angle of the incoming grain. Luckily, he's able to use metal BBs as stand-ins for sand grains in his experiments; otherwise he'd literally have to count individual grains of sand — something that not even an undergraduate can be persuaded to do.

Tran has also worked on experiments designed to determine the origin of sand ripples. Although the process of ripple formation is known in outline, many of the details remain to be worked out. A ripple starts to form when, by chance, there's a small bump on the surface. Since the wind drives saltating grains into the surface at an oblique angle, a larger number of impacts will occur on the windward side of the bump than on the leeward side. So there will be a bigger flux of sand on the windward side, sand will begin to accumulate, and the ripple will grow. It's still unclear, however, what determines how high a ripple will get or what causes the regular "wavelength" that's characteristic of a succession of ripples. Haff and Tran are trying to answer these questions using both experiment and computer simulation.

Although Haff insists "I'm doing ripples because they're fun," his work does have some practical applications. For one thing, ripples are occasionally preserved in lithified dunes. By studying "fossilized" ripples, geologists can determine the direction and velocity of ancient winds. And a better understanding of saltation will help us understand the growing problem of desertification. Many of the substances that make arable land arable are dust-sized, but it's difficult for this fine dust to enter suspension and be carried away unless it's first thrown into the air by the violent impact of a saltating sand grain.

Practical applications clearly take a back seat to aesthetic considerations when Haff discusses his interest in sand. He compares sand ripples to the rainbow. "If we didn't know where the rainbow came from, it would be something that a lot of people would be thinking about. Nobody needs a rainbow, but there it is — it's so neat that we ought to understand how it works. Sand rippling is one of those neat things that any child would notice and wonder about, but which we have no explanation for." $\Box - RF$

Zoo Story

SENIOR KARYN BETZEN spends her summer days at the Los Angeles Zoo watching the animals. The recipient of one of this year's two off-campus SURFs, Betzen is serving as an animal behavior research intern, observing gorillas and alligators under the supervision of Dr. Cathleen Cox, the L.A. Zoo's research director. Betzen's gorilla studies are part of the zoo's crucial captive breeding program and her alligator work may help bring peace to the troubled alligator pond.

The pond is the home of six American alligators — a large male named Methusela and five smaller females. Recently, the zoo keepers began noticing an increased level of fighting among the alligators, fighting that has caused the deaths of four alligators. Betzen's assignment is to try to determine the cause of this discord. "I go out every half hour and I map where they are and what state they're in: are they swimming around, are they asleep, are they drowsy, or are they awake and just sitting there? They're most active early in the morning, between 8:30 and 10:00. If they're moving around and if they're interacting with each other, I stay out and watch the whole thing until they settle down again."

After about 10 days of doing this, Betzen discovered that it was one of the females, appropriately named Bad Temper, who was causing the problem. "It's as if she's saying, 'Okay, this half of the pond is mine. And you five can share the other half.' The keepers are pretty sure it's territoriality, but I'm not entirely sure. She could have some hormonal condition that's making her edgy. She seems to be awake most of the time while the others seem to be asleep half the time. This may indicate that there's something biologically wrong with her." The keepers plan to place some logs in the pond in order to block direct access to one section. This will decrease the amount of



territory that Bad Temper can lay claim to. If this doesn't reduce the aggressive behavior, Betzen's hormonal hypothesis may well be correct.

Betzen's alligator project is pretty much her own, but she is also one of several people observing the zoo's gorillas. She's concentrating on an exhibit that houses four lowland gorillas: Tzambo, an adult silverback male; Lina, an adult female; Leo, an adolescent male; and Evie, an adolescent female. Tzambo was born in the wild. but Lina and Evie were born at the L.A. Zoo and Leo was born in captivity in Texas. Captive breeding of gorillas is a notoriously difficult task, but it may be the gorilla's only chance for survival. Says Betzen, "In the wild their numbers are dwindling fast. Their habitat is being industrialized very quickly. The future doesn't look good for them out there."

It's not known exactly why gorillas are so difficult to breed in captivity. "Sometimes the males tend to be shy," says Betzen. "If they're not reared in the wild, they've never seen other gorillas mate and so they don't know how. Also, a lot of times in captivity the males have low sperm counts, so even if they do mate the females don't get pregnant."

Betzen conducts four hours of concentrated gorilla observations each week. She comes armed with a cassette player with headphones that

keeps her informed of the time and a clipboard to record her observations, and she spends 15 minutes recording the behavior of each of the gorillas. Among other things, she records how the gorillas relate to each other and she looks for signs indicating that a female has become sexually receptive. "The hardest part is weeding out when the gorillas are interacting with the audience, when they're doing something that they wouldn't ordinarily do. Leo hams it up for the audience. He'll throw leaves on his back, which is a thing gorillas do, but he'll be doing it because people are looking at him and laughing. Evie can pick out observers. I don't know if she knows me personally, but she can always tell observers by the headphones. She'll come up to the edge and blow me a kiss."

Betzen expects this summer's experience to be extremely valuable since she plans to apply to veterinary schools in the fall. She says that she's learning a great deal about the difficulties of doing behavioral research. One problem she continually encounters is the dearth of reliable information on the animals she studies. One reference work she found asserted that only male alligators bellow. But the only alligator that Betzen has witnessed bellowing was a female. In frustration she says, "It's hard to do research on alligators. A lot of what you read about them is not true." $\Box - RF$

Emeritus Professors — 1985

ROBERT B. LEIGHTON has been a Techer for almost half a century. He entered the Institute as a junior in 1939, and received his bachelor's degree in 1941, his MS in 1944, and his PhD in 1947. He spent the next two years as an Institute research fellow, was appointed assistant professor of physics in 1949, and professor of physics in 1959. From 1970 to 1975 he served as chairman of the Division of Physics, Mathematics, and Astronomy. He was a staff member of the Hale Observatories from 1963 to 1980, and has been a staff member of the Owens Valley Radio Observatory since 1976. In 1984 Leighton was named the William L. Valentine Professor of Physics.

Leighton has made significant contributions to several scientific disciplines. Working with Nobel laureate Carl Anderson in the 1950s, Leighton built a trailer-mounted cloud chamber, which was operated at an altitude of 10,000 feet near White Mountain to capture a maximum number of the elusive "V-particles" found in cosmic rays. In 1960 Leighton developed two cameras that led to great advances in solar physics. He used the Zeeman camera to detect and map magnetic field patterns around sunspots and the Doppler-shift camera to reveal the large network of convective currents - the "supergranulation" — flowing across the sun's surface.

During the early 1960s, Leighton collaborated with Gerry Neugebauer in designing and building an innovative infrared telescope. This telescope revealed, for the first time, youthful stars hatching out of dark molecular clouds as well as aging red giants on the verge of collapse. During this time, he was also the team leader for a series of television experiments performed on some of the Mariner missions to Mars. More recently, Leighton has been pursuing millimeter and sub-millimeter wave astronomy. In collaboration with other Caltech researchers, he designed and built the three radio telescopes at Owens Valley.

And together with Thomas G. Phillips, he designed another such "dish" that's currently being installed on Mauna Kea in Hawaii.

Leighton has been elected a member of the National Academy of Sciences and a Fellow of the American Academy of Arts and Sciences. He edited the first volume of *The Feyn*man Lectures in Physics and is the author of Principles of Modern Physics and Introductory Lagrangian and Quantum Mechanics in addition to numerous scientific articles. \Box

TANS W. LIEPMANN has been at Cal-Ltech just about as long as Bob Leighton. After receiving his PhD at the University of Zurich, Liepmann came to Caltech as a research fellow in 1939. He was appointed assistant professor in 1945, associate professor in 1946, and professor in 1949. Since 1972 Liepmann has been the director of the Graduate Aeronautical Laboratories at Caltech (GALCIT). In 1976 he was named the Charles Lee Powell Professor of Fluid Mechanics and Thermodynamics and in 1983 he was named the first Theodore von Kármán Professor of Aeronautics.

Liepmann is recognized as one of the world's outstanding researchers in the field of fluid mechanics and as a notable contributor to modern aviation. During the 1940s, he and his students studied questions of boundary layer flow stability and transition, turbulent shear flow, and trans-sonic flow and shock waves. In the 1950s he performed pioneering studies of aircraft buffeting, magnetohydrodynamics, and plasma physics, work that was important in the development of supersonic aircraft. More recently his research has concentrated on problems of turbulent mixing, which is leading to the development of a new generation of engines with more efficient combustion, and to the development of highenergy chemical lasers.

Liepmann is renowned for his teaching abilities, and was the recipient of the ASCIT Award for Excellence in Teaching in 1976. His salutary influence on the graduate students who studied with him is demonstrated by the fact that 10 of his PhD students are members of the National Academy of Engineering and two are also members of the National Academy of Sciences. Liepmann himself has been elected to membership in the NAE, the NAS, and the American Academy of Arts and Sciences, and is an honorary member of the Indian Academy of Sciences. Among his many other honors and awards are the Ludwig Prandtl Ring from the German Society for Aeronautics, the Monie A. Ferst Award from Sigma Xi, and the Michelson-Morley Award from the Case Institute of Technology. □

JULIUS MIKLOWITZ received his BS, MS, and PhD degrees from the University of Michigan. After serving as a research engineer for the Westinghouse Research Laboratories, as an assistant professor of mathematics and engineering at the New Mexico Institute of Mining and Technology, and as a consultant for the Naval Undersea Warfare Center, Miklowitz came to Caltech as an associate professor of applied mechanics in 1956. He was named professor of applied mechanics in 1962.

Throughout his career, Miklowitz's research has concentrated on the pro-



Robert B. Leighton









Hans W. Liepmann

perties of elastic waves propagating through solids. He uses an analytical method he developed to solve nonseparable elastodynamic problems involving the dynamic response of elastic waveguides, wedges, and the quarter plane. Such information is important in the fields of seismology, analytical and structural mechanics,

and earthquake engineering. In one study, for example, Miklowitz investigated the effects of a nearby nuclear explosion on underground shelters or missile silos. Such an explosion produces a powerful shock wave traveling at thousands of miles an hour that radiates in all directions through the air and ground. As the ground wave sweeps around and past a subterranean cavity, it imparts its energy to the cavity wall. Part of this energy is converted into the shortperiod, intense waves known as Rayleigh waves, which circle the cavity walls at high velocities. This "bellringing" effect persists longer than the original shock wave and the reverberations can damage walls, instruments, and other structures attached to walls.

Miklowitz is the author of over 50 scientific papers as well as the book The Theory of Elastic Waves and Waveguides. He is the co-editor of the book Modern Problems in Elastic Wave Propagation (the proceedings of an IUTAM symposium) as well as the editor of an ASME monograph entitled Wave Propagation in Solids. He has been chairman of the Applied Mechanics Division of the American Society of Mechanical Engineers and has served as a member of the U.S. National Committee of Theoretical and Applied Mechanics, representing ASME. 🗆

Julius Miklowitz

Herbert J. Ryser

Nicholas W. Tschoegl

Herbert J. RYSER died on July 9 of this year, a few days before his 62nd birthday and shortly before he was to assume emeritus status. Ryser grew up in Milwaukee, Wisconsin and received his BA, MA, and PhD degrees from the University of Wisconsin. He spent a year at Princeton's Institute for Advanced Study before joining the faculty of Ohio State University. He became a professor at Syracuse University in 1962 and moved to Caltech in 1967, to become professor of mathematics.

Ryser was a major contributor to the field of combinatorics. He is best known for proving a theorem that has come to be called the Bruck-Ryser theorem. This is a classic result about sets and their intersections. He proved many other theorems as well, and his monograph *Combinatorial Mathematics* was in part responsible for a renaissance in this field of study.

Ryser was widely regarded as an excellent teacher. He taught courses in combinatorics and matrix theory at the graduate and advanced undergraduate level. His well-organized lectures and his genuine concern for his students earned him two ASCIT Awards for Excellence in Teaching. \square

NICHOLAS W. TSCHOEGL was born in Zidlochovice, Czechoslovakia in 1918 from Austro-Hungarian parents and received BSc and PhD degrees from the University of New South Wales in Sydney, Australia. After serving short stints at the University of Wisconsin and the Stanford Research Institute, Tschoegl joined the Caltech faculty in 1965 as associate professor of materials science. In 1967 he was appointed professor of chemical engineering.

Tschoegl's research interests focus on the relationship between the physical properties of polymers and their chemical and physical structures. Part of his research is concerned with novel kinds of rubbers called "block copolymers," which are two-phase systems containing a hard, glassy polymer embedded in a rubbery matrix. He and his group have taken measurements of the dynamic mechanical properties of block copolymers and have determined the superposition of the effects of time and temperature on such two-phase systems. Tschoegl has also determined the factors governing the superposition of time, temperature, and pressure effects in conventional rubbers. As a result of this work, the behavior of a rubber can now be predicted at any pressure if, in addition to certain material parameters, its behavior at atmospheric pressure is known.

But Tschoegl's interests go well beyond the horizons of chemical engineering. He has long been interested in languages, especially the Chinese pictographic language. Archaeology is another of his passions. He has delighted several Caltech audiences with talks on these subjects. One of the most popular was a Watson lecture on the archaeological reality behind the legend of Atlantis.

Tschoegl is the author of many scientific papers and was the recipient of the Senior U.S. Scientist Award from West Germany's Alexander von Humboldt Foundation. □



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Opinion

by Ned Munger

Munger teaches African politics at Caltech. The author of eight books, he recently left on his 70th visit to Africa.

THREE YEARS AGO, NONKUluleko I Nyembezi, a young Zulu woman from Durban, was admitted to Caltech for graduate study in electrical engineering. Before she could come, her UN scholarship was canceled. Upon inquiry I was told that the revolutionary forces didn't want the money spent on her, because she wouldn't help the revolution much a) as a woman, b) as a scientist, and c) because she was planning to return to South Africa. It made me angry. It was not easy to secure her the funding. Now that she has her MS from the Institute, Nyembezi may become the first black South African woman to earn a PhD in science.

When I think of some of the vehement critics of American policy toward South Africa, who gave me no encouragement in raising funds for this student's education, I have to question the sincerity of some protesters. Some shout that the time for constructive action has passed and only destruction



is to be encouraged. I challenge that.

The temptation to rush to the conclusion that South Africa is blowing up or will do so shortly has an honorable lineage. Since 1921 it has been regularly predicted that "next year South Africa will explode." In 1960 the Observer's Colin Legum, the most respected British analyst of South Africa, set 1968 as the last year to which the white regime might possibly survive. Obviously, no one can predict these things with much certainty. But despite the bad record of such predictions, I am reasonably confident that within five years the territory comprising South Africa will be governed with the consent of the majority of its inhabitants. What is cloudiest in my crystal ball is whether we will see the tragic loss of 1,000 or 500,000 lives.

Is there any chance of avoiding a Götterdämmerung? My affirmative answer is based on 40 years of friendships with black and white South Africans. Peaceful change depends on both. It is not generally appreciated that the so-called *verligte* (enlightened) movement has had strong support from key generals, who tell the politicians that there is no military solution for them in the long run. All the might of South African armaments can only buy time for the political leaders to reach an accommodation.

In my judgment, the great majority of key Afrikaners are prepared to abandon every vestige of racial discrimination. But I believe that a majority of these leaders secretly hope to maintain their power over events. History offers many examples of a minority giving up legal power but maintaining a grip over events. To me this is a false hope, but still the scrapping of apartheid would be real. I agree that changes in desegregating airplanes, restaurants, beaches, sports, and higher education do not go to the heart of the matter. The dynamic growth of black and integrated trade unions, however, is politically potent and cannot be dismissed as cosmetic.

If I am correct, and if the key Afrikaners now want seriously to discuss the salvation of all South Africa, they face the dilemma that there are few blacks who will talk to them. I know many blacks prominent in business, teaching, and government who are, frankly, afraid that when they talk to the government (and they do), they risk their homes and families going up in flames. Alan Paton, South African author (*Cry, the Beloved Country*) and co-founder of the Liberal Party, correctly pointed out the danger 40 years ago when he wrote that "when the whites have turned to loving, the blacks will have turned to hating."

I am glad that more Americans are showing a deeper concern for events in South Africa because that concern may be translated into lives saved. On a local level, a survey of Caltech attitudes by students Lisa Skrumeda and Steven Loyola revealed serious concern about South Africa among both students and faculty. They found that undergraduates, however, while most outspoken, were the least interested in making any personal sacrifice.

When I stayed with him recently in Natal, Paton suggested that Americans redouble their efforts to help black education in South Africa. Paton recalled that during the worst riots in the American South, white liberals never abondoned black education.

Two Caltech students are doing something positive. Kathleen Fletcher (biology) and Robin Whitt (applied physics) volunteered as teaching assistants at the predominantly black but racially inclusive University of the Western Cape. With the help of Caltech friends I organized the Cape of Good Hope Foundation to enhance the quality of education and reinforce the autonomy of that university. Can such volunteer efforts influence decisions in South Africa? Perhaps not, but rather than remaining neutral in a crisis, I prefer to be positive for a change. 🗆



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