Chemistry

Mirror-image threesomes in water molecules

For all its global importance, water still defies thorough understanding. Scientists cannot explain many of the properties of this ubiquitous liquid, especially on a molecular scale. Thus, they cannot fully assess the role it plays in living and nonliving systems.

Until recently, scientists lacked the far-infrared lasers necessary to study the vibrational energy of the bond that exists between the hydrogen atoms of two water molecules. But with a technique called far-infrared vibration-rotation-tunneling spectroscopy, researchers have begun to pry into the secrets of these weak forces that keep water molecules together.

"Our approach is to build up liquid water one molecule at a time," says Richard J. Saykally, a physical chemist at the University of California, Berkeley. Most recently, he has examined three water molecules cooled to the equivalent of 4 kelvins. That temperature quenches any movement caused by thermal energy, making it easier to study the quantum mechanics of this triplet.

The triplet arranges with each oxygen and three hydrogen atoms forming a six-member ring along a plane. Two hydrogen atoms stick up from this ring and one hangs down. However, each triplet quickly and continuously flips back and forth between two mirror-image configurations, Saykally and Berkeley graduate student Nick Pugliano report in the Sept. 25 SCIENCE. The up-hydrogen atoms then face down and vice versa.

This motion occurs because of a quantum effect called tunneling, which allows each water molecule to rotate around the hydrogen bond that links it to a neighboring water molecule, Saykally explains. He suspects that larger clusters of water will also exist in right- and left-handed, or chiral, forms and wonders whether water's chirality may have played a role in encouraging chirality in more complex natural molecules.

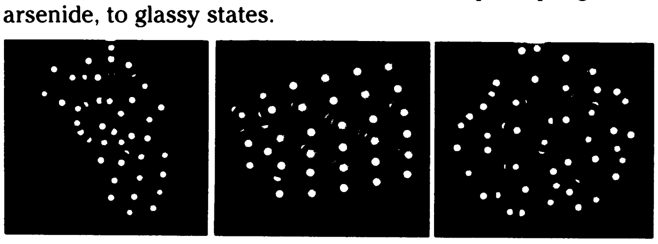
Glasses that only a computer can make

To create a glassy material from clusters would be to make the most disorderly solid possible — one that could exhibit all sorts of unexpected properties, says R. Stephen Berry, a chemist at the University of Chicago.

Berry asked his computer to do just that by cooling 32-molecule clusters of potassium chloride as fast as necessary to turn them into glass. This simulation generated a billion structures, all possibly represented in the glassy material, he reported last week in Chicago at the Sixth International Symposium on Small Particles and Inorganic Clusters.

To achieve such variety, scientists would need to cool the molecules a trillion degrees Celsius per second — 1,000 times faster than can now be done. "If you had the computer try to make it into a glass by cooling it at a rate possible in the lab, you'd never make a glass," Berry says.

But he doesn't mind. Berry simulated the salt clusters for two reasons: to try to develop efficient ways of analyzing data generated about clusters that size and to determine the forces that make the creation of glassy states so difficult. With this salt now simulated, he plans to model the conversion of magnesium, calcium, and barium oxides, and perhaps gallium arsenide, to glassy states.



Berry/Univ. of Chicago

Three simulated "glassy" clusters.

Science and Society

Problems with federal R&D priorities?

To address "increasingly urgent policy dilemmas and societal challenges" — from homelessness and AIDS to declining economic competitiveness in global markets — Congress must improve strategies for linking federally funded basic and applied research to national needs. Or so argues the *Report of the Task Force on the Health of Research,* released last month.

Rep. George E. Brown Jr. (D-Calif.), chairman of the House Committee on Science, Space, and Technology, convened the task force last year (SN: 5/25/91, p.324). Its mission: to probe widespread reports of stress in the federally funded research system and investigate how Congress might relieve that stress.

Increasingly, federal research investments are failing to deliver the dividends that Congress and the public have come to expect, Brown says. The problem reflects not waning research quality, he contends, but a growing divergence in the goals of those who have tended to set federal research agendas — scientists — and those who have paid for the research. While scientists have been aiming for a greater understanding of how the world functions, most taxpayers have supported these programs as a defense against military or economic aggression.

The task force found that Congress tends initially to base its research-funding decisions on the promise that a particular line of inquiry offers. The new report recommends that Congress now consider adding a performance review — by independent auditors — of programs it finances. Congress should also issue "a clear statutory mandate to redirect or terminate programs that are not making sufficient progress toward stated goals," the task force says. And it suggests that policymakers articulate research goals more clearly and centrally, from outside the parochialism of individual federal agencies, as the new FCCSET (Federal Coordinating Council on Science, Engineering, and Technology) programs do.

Similar conclusions emerge from another research and development (R&D) analysis, this one contained in a 318-page report titled "Setting Domestic Priorities," released last month by the Brookings Institution in Washington, D.C.

Like Brown's task force, Linda R. Cohen of the University of California, Irvine, and Roger G. Noll of Stanford University found that federal R&D investments reflect "many uncoordinated decisions rather than a comprehensive policy" and are subject to little accountability, such as whether they are meeting objectives. Overall, Cohen and Noll argue, the main problem "is not *how much* [the United States] invests, but how it sets priorities and how it manages what it spends."

For instance, they note that while the United States spends about the same fraction of its gross national product on R&D as other industrial nations do, "nearly all of the [U.S.] R&D effort goes to defense, health, and energy." No major industrial competitor focuses as extensively on these areas, they say — nor, probably, should the United States.

Noll and Cohen also explore a range of political and economic factors that could impede major reforms in federal R&D priority setting. For instance, killing programs that don't meet targeted objectives or embracing new technologies may render some labs, companies — even entire industries — instantly obsolete. Count on "losers" exerting political pressure to sustain these dying programs, Noll and Cohen say.

They also note that civilian technology "rarely" wins federal funding, largely because innovation occurs so slowly, its results are uncertain, and its ultimate beneficiaries have proved hard to predict. "Unless the United States overcomes its political resistance to supporting civilian R&D without a strong national security justification, the gap in civilian R&D between the United States and its principal international competitors is likely to widen," they conclude.