Coming 'round to old views of benzene

A new view of the electronic structure of benzene comes nearly full circle to a 121-year-old vision of the molecule. In 1858 Friedrich August Kekulé introduced his valence bond theory of chemical combination that he used in 1865 when he suggested a chemical structure for benzene. He argued that the then anomalous chemical properties of benzene were somehow due to the ability of benzene's double bonds to oscillate between two six-carbon ring structures that were identical save for a shifting of the three double bonds.

Had Kekulé known in his time about quantum theory's concept of molecular orbitals introduced in the late 1920s, he would have melted his two structures into what is now called a "resonance hybrid." Molecular orbital theory, which accounts for chemical bonding by describing where electrons are likely to be found around a molecule, is presented in today's general chemistry courses as a modern refinement of Kekulé's valence bond theory, which describes how electrons localized around atoms interact to form bonds. Modern theory draws a picture of benzene in which delocalized electrons dash about in dough-nut-shaped orbitals above and below the entire ring of six carbon atoms.

Now, using a revised valence bond theory that incorporates electronic spin, new calculations of benzene's electronic structure reported in the Oct. 23 NATURE by David L. Cooper of the University of Liverpool, Joseph Gerratt of the University of Bristol and Mario Raimondi of the University of Milan indicate that the "delocalized" electrons of molecular orbital theory are actually localized in deformed orbits about the individual carbon atoms. They comment in their article that Kekulé's 19th century views on the matter come closer to this newest picture of benzene than to the benzene of molecular orbital theory.

New symbols for reaction mechanisms

During a chemical reaction, bonds between atoms are made and broken. For over 30 years, chemists have been using symbols devised by Sir Christopher K. Ingold for categorizing reactions according to patterns of bond transformations. These symbols consist of a limited cast of letters and numbers that represent chemical events such as an atom substituting for another on a molecule, the elimination of a group of atoms from a molecule and how many molecules "touch" during a particular reaction. But Ingold's system "has become unwieldly and, in some cases, ambiguous," says Robert D. Guthrie of the University of Kentucky in Lexington.

At regional offices of the International Union of Pure and Applied Chemistry (IUPAC), chemists soon will be able to review a proposal for a new system of symbols for chemical reactions that a high IUPAC official says is "more rational and comprehensive" than Ingold's system. The new system, which was proposed by Guthrie in 1975 and has since been refined by an IUPAC committee of which he is a member, will probably be approved by the IUPAC at the end of next summer. Guthrie argues the new symbolic system is a "more logical approach" to describing reaction mechanisms that is "closer to how organic chemists think." He says that the symbols — a refined set of numbers, letters and punctuations — describe more clearly the sequence of bond making and breaking during chemical reactions. Furthermore, Guthrie says that simply using the new symbols could stimulate researchers to ask important experimental questions that they would otherwise overlook.

Joseph Bunnett, president of the organic chemistry division of IUPAC, says the new system is "sailing smoothly" through the organization's involved approval process. Just how far the system gets once it is approved will depend more on how effectively Guthrie and the IUPAC commission can market it, Bunnett adds.

Progress in the African locust wars

An "unprecedented level" of cooperation between donor nations and African states in fighting locusts and grasshoppers has averted the threat of famine in much of Africa, according to the United Nations Food and Agriculture Organization (FAO). The continent has been plagued this year by the worst swarms of locusts and grasshoppers in many decades (SN: 8/16/86, p.105). More than 500 tons of pesticides — donated by the United States, Japan and European nations — were used to save an estimated 90 percent of the crops threatened by swarms of Senegalese grasshoppers in West Africa. The pesticides, together with good weather, also reduced the risk of massive crop devastation in East Africa from African migratory locusts and red locusts, FAO says.

The agency reports, however, that the brown-locust outbreak in southern Africa, now in its second year, remains unchecked. Complicating control measures in that region is the large range of the pest — 40 million hectares.

Defense not hurting engineer supply

Almost 70 percent of federal research and development spending goes for defense (SN: 2/15/86, p.100). Because the industrial defense sector is also expanding, there has been concern that these programs might be siphoning off most of the nation's best young engineers, and setting up the civilian sector for a serious shortfall of available engineering graduates — a factor that could affect U.S. industrial competitiveness. But a new study by the National Academy of Engineering in Washington, D.C., indicates such fears are largely misplaced. It found that the United States' defense buildup has "not seriously affected" the number of engineers available to the civilian sector.

Placement officers from about a dozen academic institutions told the study's authors that today's overall demand for graduates roughly matches supply and that graduates are less averse to working on defense projects now than during the late 1960s. In fact, the report found, jobs in the defense sector "have acted to offset declines in recruiting activity by the commercial sector and to absorb increases in the supply of engineering graduates." However, the study notes, there is still a serious shortage of engineering faculty, and defense programs may generate civilian labor shortages in some specialties — like optics.

Legislative briefs

• The Asbestos Hazard Emergency Response Act (SN: 10/25/86, p.264) became law on Oct. 22. In addition to providing timetables and standards for dealing with asbestos in some 35,000 schools, it requires the Environmental Protection Agency not only to assess over the next year the extent to which asbestos-containing materials in public and commercial buildings threaten public health, but also to determine whether a program for inspection and remedial action — similar to that now in place for schools — should be developed.

• President Reagan used his pocket veto on Nov. 2 to kill the proposed National Energy Conservation Act of 1986, a bill that would have set federal energy efficiency standards for consumer appliances.

• The President also pocket vetoed the Clean Water Act Reauthorization on Nov. 6. He wanted the bill to authorize only $6 billion for sewage treatment over 4 years, not the bill's proposed $18 billion over 9 years. The bill would also have set up a new program to control the runoff of toxic chemicals, including pesticides, from such non-industrial sources as farms and construction sites. "It's astounding that a concern at the top of the public environmental agenda would be ignored by the White House," says Sharon Newsome of the National Wildlife Federation, which lobbied for the bill's passage. The bill had also won unanimous House and Senate approval (SN: 10/25/86, p.264).

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