Chemistry

The electronic look of explosives

Chemical explosives with similar molecular structures often show great differences in their sensitivity to shock waves used to detonate them. One such group is the nitroaromatic explosives, which includes compounds such as trinitrotoluene (TNT) and triaminotrinitrobenzene (TATB). These explosives have a molecular structure consisting of an aromatic or benzene ring of six carbon atoms to which nitro (NO_2) and sometimes other chemical groups are attached. Depending on the specific molecular arrangement, the pressure needed to initiate an explosion varies by as much as a factor of five.

Recently, a team of scientists at the Sandia National Laboratories in Albuquerque, N.M., led by J. William Rogers Jr., used a sophisticated technique known as X-ray-excited Auger electron spectroscopy to investigate in detail the arrangement of electrons in molecules of these explosives. The "soft" X-rays, unlike electron beams, are gentle enough to excite electrons within the material's atoms without causing the explosive to detonate. The technique allows the researchers to look at the energy levels associated with bonds between carbon atoms.

Their analysis confirms theoretical predictions that the addition of nitro groups weakens the carbon-carbon links in the aromatic ring. This makes molecules with nitro groups easier to break apart and hence more sensitive to shock waves. If amino (NH_2) groups are also present, the compounds are more shock resistant. The amino groups seem to strengthen carbon-carbon bonds by adding to their electron density. Moreover, this redistribution of charge makes amino groups slightly positive and any nitro groups present slightly negative. As a result, molecules having both nitro and amino groups can attract one another to form a network. This network absorbs some of the energy carried by a shock wave, reducing the amount of energy reaching the ring itself.

Overall, the Sandia studies show that the stability of the carbon ring is at least partly responsible for shock sensitivity. However, macroscopic properties such as particle size and shape and the material's density also play important roles. A full understanding of how explosions are initiated is likely to come only after the interplay between microscopic and macroscopic effects is studied.

Reviving an old route to chlorine

A chemist at the University of Southern California in Los Angeles has devised a process that promises to cut the cost of converting hydrochloric acid to chlorine. Chlorine is widely used for producing substances such as laundry bleaches, dry-cleaning fluids and industrial solvents. However, one of the by-products of manufacturing these substances is hydrochloric acid. Because hydrochloric acid has only a limited number of uses industrially, disposing of the excess has been a significant problem.

Chemist Sidney W. Benson and researcher Mohammed Hisham have found an economical way to convert hydrochloric acid into additional chlorine. Their method is a variation on a technique first devised in 1865 by chemical engineer Henry Deacon. Deacon's process involves burning hydrochloric acid in oxygen or air to produce water and chlorine. But the process is slow, and raising the temperature to speed it up encourages the reverse reaction of chlorine with water to give back oxygen and hydrochloric acid. Deacon proposed using a catalyst, but the resulting mixture of products was difficult to separate.

Benson avoids the problem by altering the way in which the reaction is done—by changing the order of steps and the type of equipment used. Because his recipe has potential industrial applications, Benson is not yet ready to reveal its details publicly.

Earth Sciences

Ice traces of catastrophe: Chernobyl . . .

Frozen into the earth's ice sheets is a rich history of the changing composition of atmospheric gases, the planetary wind patterns and varying snowfall rates. But to unlock these records, scientists need to know the dates at which layers of ice were created. In this respect, the cloud of the April 1986 Chernobyl nuclear reactor accident had a silver — or rather, a cesium — lining.

Cliff I. Davidson at Carnegie-Mellon University in Pittsburgh and his colleagues report in the Aug. 7 SCIENCE that "a well-defined layer of radioactive cesium is now present in polar glaciers, providing a new reference for estimating snow accumulation rates and dating ice core samples." Because the Chernobyl cloud extended only into the troposphere (where, within weeks, particles either fall out or are washed out with precipitation), it left a much clearer signal in the ice than did past nuclear weapons tests, which spewed radioisotopes into the stratosphere where residence times exceed a year.

By matching the temperatures at which ice layers form (as determined by the ratios of oxygen isotopes) with meteorologic temperature records, the researchers got a good idea of when and how most of the cesium-137 and cesium-134 arrived on the ice sheet. They also found, with the aid of cesium measurements made elsewhere and with a computer model of wind patterns, that the Chernobyl cloud spread uniformly across North America. "That tells us that what we measured in Greenland," says Davidson, "other scientists are probably going to be able to measure wherever they go in the Arctic."

. . . and the ancient volcano Thera

Radioactive emissions from nuclear testing and accidents are not the only events that create geological reference markers. By ejecting ash and debris into the atmosphere, volcanoes also leave their mark. The violent eruption of the Aegean island of Thera (or Santorini) about 3,500 years ago left an important legacy not only for geologists but for archaeologists as well, because it buried a number of developing Bronze Age settlements on the island and is thought to have wiped out the Minoan civilization on Crete, to the south.

Unfortunately, although Thera's debris long ago settled to ground, the exact date of its eruption remains up in the air. By comparing Thera's cultural development with that found elsewhere, most archaeologists have placed the eruption at about 1500 B.C., whereas radiocarbon dating of shrubs and other objects suggests dates more than 100 years older. In the Aug. 6 NATURE, Danish researchers present the results of yet another method, which produced dates slightly older than the radiocarbon studies. C.U. Hammer at the University of Copenhagen and colleagues searched for acidity peaks in South Greenland ice cores. They found one layer containing high levels of sulfuric acid (which is formed from volcanic sulfur dioxide), and by counting seasonal variations in snow deposits, they conclude that Thera erupted in 1645 B.C.

Seismic signals of a meteor wave

In the early morning hours of Sept. 19, 1986, a resident of Yellowknife, Northwest Territories, saw a meteor streak by overhead. Frank M. Anglin and Raymond A. W. Haddon at the Geological Survey of Canada in Ottawa report in the Aug. 13 NATURE that they subsequently found seismic signals at the Yellowknife seismic array that were probably generated by the shock wave created by the meteor as it moved through the atmosphere. There have been two previous reports of seismically detected meteors, but the researchers write that theirs is "the first unambiguous [observation] of a shock wave and associated seismic waves generated by a meteoroid and observed by an array of closely spaced seismometers."