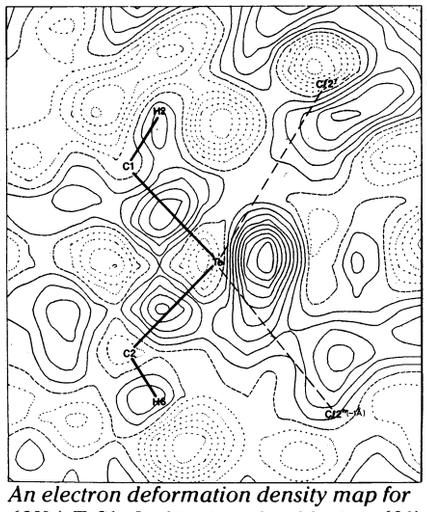
Charting 'deformed' electrons of a heavy

The groups of electrons that surround atoms are like balls of chewing gum. Left to their own devices, the groups tend to stay spherical. But when the atoms they surround are attracted and bond to other atoms, then the shape of these groups changes — just as the spheres of gum are distorted when two are brought together and then pulled slightly apart. While most of the electrons remain in the spheres, some end up stretched out between the two main masses.

Scientists understand fairly well the behavior of the electrons that remain in spherical regions. "There's not much mystery about where they are located," says Jan M. Troup of Molecular Structure Corp., in College Station, Tex. However, the nonspherical region electrons are less understood, and their precise behaviors and locations must be elucidated before scientists can fully comprehend what goes on when atoms bond.



Ziolo and Troup/JACS

An electron deformation density map for $(CH_3)_2TeCl_2$. In this view, the chlorines (C1) are from a neighboring $(CH_3)_2TeCl_2$.

Now, in research that has shined more light on these nonspherical regions, Troup and colleague Ronald F. Ziolo of Xerox Corp., in Webster, N.Y., have generated special electron maps of the heavy-atom molecule dimethyltellurium dichloride $(CH_3)_2TeCl_2$. (Xerox and other copy machine manufacturers use tellurium, Te, alloys in their equipment.)

The maps, described in the Jan. 26 JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, are pictures of the "electron deformation density" — the amount of negative charge from the nonspherical (deformed) region electrons per given area of space — of the tellurium molecule. Rarely have these maps been generated for molecules that contain such a heavy atom (the atomic number of tellurium is 52). In fact, due to the large potential for error in studies that involve weak electronic signals from the nonspherical regions of heavy atom-containing molecules, such mapping until now has been confined mainly to compounds and materials containing atoms with atomic numbers less than 30, Ziolo and Troup report.

The researchers say they owe their success to several factors, including use of high-quality tellurium compound crystals during the first step toward a density map: an X-ray crystallography experiment. In this step, X-rays beam the crystal; how they diffract reveals structural information about those crystals. That information in turn is manipulated and combined with other data in order to generate an electron density map. Finally, the densities of the electrons from the spherical regions are "subtracted out," and what remains on the map are the "deformed," or nonspherical, region electrons.

As is the case with all electron density maps, the resulting picture resembles the contour-line topography maps on which, for example, each curve represents a specific elevation. In this case (refer to the map), each contour represents a density of negative charge at intervals of 0.03 electrons per cubic angstrom. The map confirms several bonding interactions that until now have only been suspected. For example, the group of contours centered just below and a little to the right of the C12′ on the map confirm that in the crystalline state, a weak intermolecular bond forms between the tellurium of one dimethyltellurium dichloride molecule and the chlorine of another such molecule.

Ziolo says that eventually, such electron deformation density mapping may be extended to include study of complex biologic molecules, which undergo significant intermolecular bonding. Also, he says, it should prove useful for the study of electronically important molecules, including the semiconductor material gallium arsenide. *—L. Garmon*

Runners and anorexics: An ascetic disorder?

Alberto Salazar, the marathon runner, once reportedly ran more than 100 miles a week with an unhealed stress fracture rather than break training. During one marathon, he pushed himself so hard that his body temperature rose to 108°F; he was packed in ice and treated for heat prostration while a priest gave him last rites. Such extreme commitment to athletic performance has a time-honored place in American culture, but scientists studying compulsive runners are now saying that this extreme commitment should be recognized as a self-destructive and pathological behavior. It is a primarily male manifestation of what they call an "ascetic disorder," which, in women, tends to show up as anorexia nervosa, or self-imposed starvation.

Writing in the Feb. 3 NEW ENGLAND JOURNAL OF MEDICINE, psychiatrists Alayne Yates and Kevin Leehey and psychologist Catherine M. Shisslak, all of the University of Arizona, say that while extreme dieting has been recognized as a serious emotional disorder, extreme training is viewed by society positively, as evidence of dedication. But the psychology underlying both behaviors appears to be the same.

Based on a study of 60 marathon runners, they report that the "obligatory runners" (those who are consumed by running, who run in spite of illness, and who suffer depression when they cannot run) tend like anorexics to be introverted, compliant, self-effacing and unable to express anger. Each has an unstable self-concept, and the commitment to diet or to exercise is an attempt to establish a firm sense of identity; while women tend to focus on slimness, men focus on physical prowess — both strong values in American culture. Like anorexics, compulsive runners tend to be high achievers from affluent families. And in both cases, the researchers say, the pathological commitment begins at a time of heightened stress: for females, during adolescence; for males, during middle age. The incidence of both disorders has increased dramatically over the past decade.

Anorexia is poorly understood, but one theory is that it is related to a malfunctioning hypothalamus, which controls the release of morphine-like endorphins in response to stress. Scientists have found that emaciated anorexics have elevated brain levels of endorphins, which may be associated with the elevated mood many report. The same brain chemistry has been theorized to play a role in the emotional "high" that distance runners report. The mood changes caused by increased opiate activity could serve as a potent reinforcer of destructive behavior, the Arizona researchers say.

A small minority of anorexics are male, and similarly a small number of compulsive runners are women. These women often stop menstruating (as do anorexics) before they commit themselves to running. Compulsive runners tend to be extremely concerned about their weight, the researchers note, just as many anorexics are preoccupied with exercise; nearly starved anorexics have been known to stay up all night doing jumping jacks. Both suffer from a perceptual disorder; just as anorexics continue to perceive themselves as fat when they are half-starved, runners feel out of shape long after they are dangerously overtrained. The most striking characteristic shared by both groups is what the researchers describe as "a grim asceticism and an assiduous avoidance of passive, receptive pleasures." *—W. Herbert*