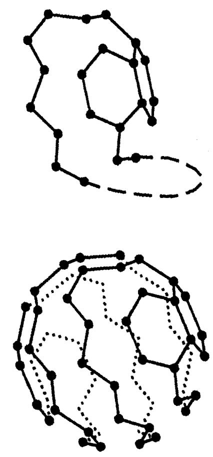
Carbon precursors wrap into buckyballs

Amid all the current hoopla surrounding the buckyball, the soccer-ball-shaped molecule from the fullerene family, chemists continue to wonder exactly how all of its 60 carbon atoms come together to make this elegant structure. Why, for instance, do the carbon atoms form a ball and not some other shape?

Now, experimental results back up a proposed explanation for this feat. Joanna M. Hunter and her colleagues, all chemists at Northwestern University in Evanston, Ill., describe a mechanism by which carbon atoms form "fullerene precursors." These subsequently wind themselves into spherical carbon cages.

Studying carbon clusters made up of 50 to 70 atoms each, the chemists find that the atoms tend first to form paired hexagonal rings, around which a long chain of carbon atoms extends. Under the right conditions, this chain will wind itself up to form the rest of the ball-shaped fullerene. Their results appear in the Feb. 17 JOURNAL OF PHYSICAL CHEMISTRY.

"We've been after a specific mechanism to explain how carbon, which naturally forms rings, will convert into a spheroidal cage. So we've been measuring the amount of energy needed to drive this structural transformation," says Martin F. Jarrold, a coauthor of the report. "We find that this transformation occurs fairly easily, driven by a remarkably small amount of heat. This efficiency appears to hold not just for C_{60} but for other carbon clusters as well."



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The proposed fullerene-forming mechanism begins when a process called Bergman cyclization causes two hexagonal carbon rings to close up, creating a "fullerene fragment." That fragment then serves as a sort of seed structure, allowing a dangling chain of carbon atoms to kink itself into other hexagons and pentagons. Once configured this way, the chain then "spirals around the fullerene fragment and zips up to form a spheroidal fullerene," the chemists explain.

"By understanding the mechanism that has these carbon rings collapse into fullerene spheres, maybe we can think about making other fullerene derivatives," says Eric J. Roskamp, another coauthor. "So this model may have practical uses, especially if you want to make a particular type of fullerene." Grasping the details of this mechanism may help chemists streamline the process by which ordinary flat carbon rings pull themselves together to form carbon cages, he adds.

Jarrold has fleshed out this model of buckyball formation by making "endohedral metallofullerenes," which house lanthanum metal atoms within the carbon cages. By zapping graphite rods and lanthanum oxide with a laser, Jarrold and his colleagues created an abundance of metal atoms trapped inside fullerenes, converting them with "remarkably high efficiency."

Based on their best results, Jarrold and his colleagues believe that the lanthanum itself is acting as a "nucleation center," around which the carbon rings arrange themselves before becoming a complete cage. These intriguing results will appear in a forthcoming NATURE. *—R. Lipkin*

Mercurial airs: Tallying who's to blame

Each year, human activities throughout the United States release an estimated 341 tons of gaseous mercury into the air, according to an Environmental Protection Agency draft report that inventories the toxic pollutant. This report constitutes the first comprehensive attempt to gauge airborne mercury releases nationwide in almost 20 years — a time during which industries that use and products that contain the metal have changed dramatically.

Fossil-fueled power plants have long been recognized as the single largest industrial source of airborne mercury. The pollutant has rendered fish throughout large portions of North America a serious threat to human health (SN: 3/9/91, p.152). The inventory links 36 percent of the anthropogenic releases — emissions from human activities — to naturally occurring mercury contaminants in the fuel used at such power plants: about 117 tons per year to trace levels in coal and 4.4 tons per year to the mercury released from burning oil.

Three other types of combustion facilities play a major role, the new EPA report notes. Every year, incinerators burning mercury-laced municipal trash and medical wastes contribute 64 tons of mercury each, it says, while commercial and industrial boilers together spew out another 30 tons of the highly toxic metal.

Though the U.S. government controls mercury releases from a select group of industries, no federal limits exist for what the inventory points to as the biggest contributors — power plants, incinerators, and other combustion sources. Together, these account for an estimated 83.6 percent of all industrial and residential mercury releases to the air. Moreover, because incinerators emit an extremely soluble form of the metal, most of the mercury they discharge can wash out of the air — and into the food chain — more effectively than can the mercury released by power plants.

But controls on some relatively big mercury polluters could emerge soon. Over the past 2 years, the Natural Resources Defense Council and the Sierra Club Legal Defense Fund (SCLDF), both in Washington, D.C., have sued EPA to force the agency to develop mercury controls for combustion facilities. Last December, EPA entered into a tentative settlement with the groups, notes Howard Fox of SCLDF.

Perhaps as early as September, EPA intends to issue revised emission standards for municipal incinerators; these will explicitly target mercury emissions. Somewhat later, the agency will propose controls for medical-waste incinerators, notes EPA's Robert Martineau. "I don't have any idea what the requirements will be," he says, "but mercury emissions will be considered."

Here the new inventory may prove helpful, argues Marjorie J. Clarke, a New York City-based consultant active in drafting state incinerator limits on mercury. A lack of data on the role of medical-waste incinerators as a source of mercury has hampered efforts to impose controls on these facilities, Clarke notes. But if, as the new inventory suggests, garbage and medical waste pose the same threat, she says, "then you would want to attack them with the same vigor."

What about power plants? Congress has charged EPA with studying mercury emissions from them. Pending results, these facilities are exempt from federal mercury controls. Under the 1990 revisions to the Clean Air Act.

Overall, the new inventory says, 40 percent of the mercury in air may trace to natural sources — volcanic eruptions and vapors from mercury-laced rocks, soil, and water. However, EPA also concedes that "natural sources" is a bit of a misnomer, since these releases include some revolatilization of "yesterday's anthropogenic emissions."

Indeed, the inventory's global figure for natural mercury emissions seems greatly exaggerated and its numbers for many industrial contributions low or absent, according to Eva Voldner, who analyzes such data for Environment Canada's Atmospheric Environment Service in Downsview, Ontario. *—J. Raloff*