Technology Networks

All-Metal Fullerene Molecule Synthesized for the First Time

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In a world-first, researchers have created a fullerene-like molecule composed entirely of metal atoms.

Synthesized by a team of chemists from China's Nankai University, Nanjing Tech University and Shanxi University, alongside a colleague from the Universidad San Sebastián, Chile, the new molecule is made up of 12 gold and 20 antimony atoms that surround a single positively charged potassium cation in its center.

While the instability of this new metal complex could limit its direct practical applications, the researchers say that its synthesis could still provide valuable new insights into the bonding behavior of metal atoms.

The researchers have described their new discovery in a paper published in the journal *Science*.

What is fullerene?

In 1985, while conducting experiments aimed at understanding how long-chain carbon molecules form in interstellar space, chemists spotted an oddity in their mass spectrometry results – a discrete peak correlating with a molecule made up of exactly sixty carbon atoms.

The research team – which included chemists Harold Kroto of the University of Sussex alongside Robert Curl and Richard Smalley from Rice University – investigated further, discovering that the oddity was a cage-like sphere made up of single- and double-bonded carbon atoms. They named this oddity "Buckminsterfullerene", after the influential American architect Richard Buckminster Fuller, who was known for his designs featuring geodesic spheres. They published their findings in a letter to the journal *Nature*.

In the following years, researchers would identify other similar molecules in this "fullerene" compound class that contained different numbers of carbon atoms. The highly symmetrical structure, distinctive physical properties and the shape-dependent chemical reactivity of the fullerenes gave rise to a broad range of potential applications, with these molecules being used in impact-resistant lightweight materials, solar cells and even in the medical field. Ultimately, the discovery of fullerenes would earn Kroto, Curl and Smalley the 1996 Nobel Prize in Chemistry.

Full-metal fullerene

Since the discovery of Buckminsterfullerene, similar inorganic (carbon-free) fullerene-type structures have been theorized. Such inorganic fullerenes are expected to have exceptional stability and reactivity, making them an attractive target for chemists.

However, the synthesis of an all-metallic inorganic fullerene has proved to be a significant challenge; quantum chemical theory suggests that a spherical Au_{32} form of gold should exist, but it has only ever been spotted when stabilized by external molecular ligands.

Now, researchers report the synthesis and characterization of the world's first all-metal fullerene. The molecule – a potassium–gold–antimony anion with the formula $[K@Au_{12}Sb_{20}]^{5-}$– was prepared by combining K_8SnSb_4 with a gold(I) phosphine complex in an ethylenediamine solution. This yielded large black crystals, which were analyzed using X-ray diffraction and energy-dispersive X-ray spectroscopy to probe the molecule's structure.

This analysis confirmed that the potassium–gold–antimony complex formed a fullerene-like dodecahedral structure, with a gold atom at the center of each face and an antimony atom at each vertex. In the very center of the molecule was a potassium atom, which coordinated with each gold atom to hold the structure in place.

The research paper notes that the molecule is extremely air-sensitive. This instability likely precludes it from being used directly in any practical applications. However, the researchers believe that the metallic bonding behavior observed in this molecule could provide chemists with valuable insight that could be used to develop more stable inorganic fullerenes, optoelectronic materials or other novel nanostructures.

Reference: Xu YH, Tian WJ, Muñoz-Castro A, Frenking G, Sun ZM. An all-metal fullerene: $[K@Au_{12}Sb_{20}]^{5-}$. *Science*. 2023;382(6672):840-843. doi: 10.1126/science.adj6491