CHEMISTRY

Keep your eye on the atom

Researchers use atomic force microscopy to image the chemical structure of the small molecule pentacene, with atomic resolution.

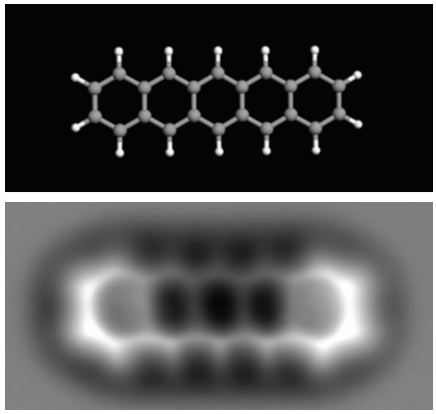
How many times have chemists wished for a microscope so powerful that they could see right down to the atomic level of an individual molecule? Scientists at IBM Research in Zurich, Switzerland have now achieved this elusive goal, using atomic force microscopy (AFM).

An atomic force microscope uses a cantilever with a sharp tip to scan the topology of a surface. In noncontact mode, the cantilever is oscillated at a specific frequency; when the tip comes incredibly close to the sample surface, the frequency shifts as a result of forces between the tip and the sample.

To obtain atomic resolution imaging of single molecules, the IBM team had to first tackle some experimental challenges. To ensure a stable operation, they used a low temperature (5 K), noncontact AFM instrument in constant height mode, with a high stiffness cantilever. They also needed to know the exact atomic composition and geometry of the AFM tip to be able to precisely interpret the force measurements; they settled on a tip terminated with a single CO molecule. Unlike a typical metal AFM tip, "The CO tip is quite inert, and it prevents the molecule [under study] from being bonded to the tip," explains Leo Gross, a scientist on the IBM Research team. This, as it turned out, was the key to obtaining atomic resolution.

Gross and his colleagues demonstrated their technique by imaging the small molecule pentacene, which consists of five fused benzene rings. The atomic resolution AFM image speaks for itself. "We didn't expect to have such high resolution," says Gross, noting that the team was surprised that they could clearly image the five rings, the bonds between atoms and even the carbon-hydrogen bonds. But they also performed density functional theory calculations, which confirmed that the pentacene images were what they should have seen.

There are of course other methods by which atomic-resolution molecular structures can be obtained, such as by nuclear magnetic resonance (NMR) spectroscopy or crystallography. But the ability to image individual molecules is unique to this AFM-based technique. With such an approach, for example, "we can say whether something happens to this one molecule; if we have a charge transfer or if we exchange one atom or dissociate one atom," explains Gross.



The atomic structure of pentacene. Ball-and-stick model of pentacene (top). AFM image of pentacene using a CO-modified tip (bottom). Image courtesy of IBM Research, Zurich; reprinted with permission from the American Association for the Advancement of Science.

Beside resolving the structures of unknown molecules, the AFM technique could be used to address a number of interesting chemical questions. Gross and his colleagues are hoping to push the approach to identify atomic species, to distinguish a carbon atom from an oxygen or a nitrogen or a sulfur atom, for example. They also believe the technique could be used to answer fundamental questions about chemical bonding, such as bond order (how many electrons are participating in a bond) and bond length.

By using a reactive molecule at the tip, researchers could also potentially use the approach to directly probe the molecule under study, perhaps leading to new atomic-level insights about chemical reactivity and catalysis. The possibility for these kinds of manipulation experiments, says Gross, "are what distinguishes AFM from other microscopy techniques."

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RESEARCH PAPERS

Gross, L. *et al.* The chemical structure of a molecule resolved by atomic force microscopy. *Science* **325**, 1110–1114 (2009).