Breakthrough in chemical crystallography

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A research team led by Professor Makoto Fujita of the University of Tokyo, Japan, and complemented by Academy Professor Kari Rissanen of the University of Jyväskylä, Finland, has made a fundamental breakthrough in single-crystal X-ray analysis, the most powerful method for molecular structure determination. The team's breakthrough was reported in *Nature* on March 28, 2013.

X-ray single-crystal diffraction (SCD) analysis has the intrinsic limitation that the target molecule must be obtained as single crystals. Now, Professor Fujita's team at the University of Tokyo together with Academy Professor Rissanen at the University of Jyväskylä have established a new protocol for SCD analysis that does not require the crystallisation of the target molecule. In this method, a very small crystal of a porous complex absorbs the target molecule from the solution, enabling the crystallographic analysis of the structure of the absorbed guest along with the host framework.

As the SCD analysis is carried out with only one crystal, smaller than 0.1 x 0.1 x 0.1 mm in size, the required amount of the target molecule can be as low as 80 ng. Fujita's and Rissanen's work reports the structure determination of a scarce marine natural product from only 5 μg of it. Many natural and synthetic compounds for which chemists have almost given up the hope of analysing crystallographically can now be easily and precisely characterised by this method.

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