Australian Government

ANSTO
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Case study: Modern structural chemistry

The pharmaceutical sector relies on accurate structure determination of their molecular materials to understand their properties and possible applications. Neutron scattering can be particularly effective in the investigation of small molecules where the location of hydrogen atom positions is paramount.

國立東華大學
National Dong Hwa University

The Chinese puzzle molecule

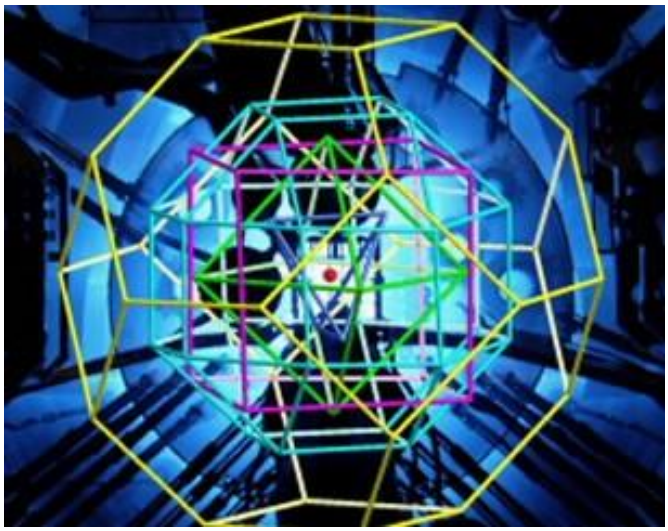
The Chinese Puzzle Molecule was brought to ANSTO through the our user programme by colleagues at National Dong Hwa University in Taiwan.

Initial X-ray studies had revealed the molecule was comprised of a complex, multi-layered structure of copper and sulfur atoms with some other atomic species showing an apparent average atomic number around Z=10. Nuclear magnetic resonance studies provided evidence for eight hydrides which were suggested to lie at the corners of a cube within the complex structure.

Using neutron diffraction it was clearly shown that these eight hydrides were present in the expected positions, but also that another six hydrides resided deeper inside the structure with a further single hydride located at the centre.

Once the presence of these hydrides was demonstrated, it was evident that the initial assignment of the twelve sites as disordered S8 based on the X-ray diffraction data was incorrect. A simple elemental analysis provided the correct assignment of these twelve sites as 1/3rd occupancy copper sites, giving an excellent fit to the neutron data.

The final model for the molecule, shown here, illustrates that the four inner copper sites lie at the corners of a tetrahedron around the inner hydride and inside the octahedron of hydride.



The $Cu_{28}H_{15}S_{24}$ assembly at the core of the "Chinese Puzzle Molecule" as revealed by single-crystal neutron diffraction.

The contribution of the Australian Centre for Neutron Scattering

The Koala Laue Diffractometer instrument was used to perform single-crystal neutron-diffraction studies which complemented the initial studies performed using X-ray diffraction and nuclear magnetic resonance.

The results of studies of this type provide researchers with data that give valuable information about the location of hydrogen atoms in a structure or can be used to differentiate elements of similar atomic number.

Such insights are fundamental to our knowledge of how compounds behave in agricultural or medicinal applications where structural binding to a biological substrate is understood at the atomic scale.

More information:

A.J. Edwards, R.S. Dhayal, P.-K. Liao, J.-H. Liao, M.-H. Chiang, R.O. Piltz, S. Kahlal, J.-Y. Saillard & C. W. Liu. Chinese Puzzle Molecule: A 15 Hydride, 28 Copper Atom Nanoball. Angewandte Chemie, 126(28), 2014. pp. 7342-7346.