

12 pentagonal $\{\text{Mo}(\text{Mo})_5\}$ clusters bridged by 30 linkers — have attracted particular attention. Now, Paul Kögerler from the Forschungszentrum Jülich and co-workers in Germany, Belgium and the US, have used Raman spectroscopy to monitor the formation of a partially reduced Keplerate system with altered intramolecular magnetic interactions.

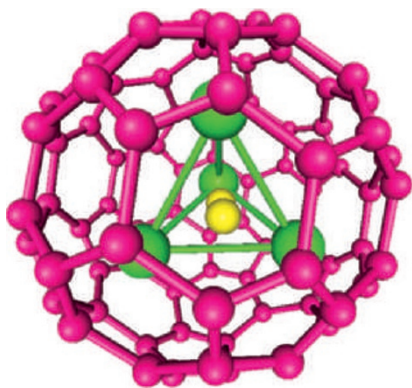
The researchers first formed Keplerate species featuring Fe-, V- and Mo-based linkers by precipitation. They then added KCl to the remaining solution before leaving it exposed to air for two weeks, which led to the partial reduction of the Mo(VI)-based units. The Keplerate clusters that were subsequently collected by precipitation were shown to be Mo(V)/Mo(VI)-based clusters linked only by iron-based units.

These clusters had a similar structure to that of previously reported Mo(VI)-based clusters, but were highly charged. They therefore stacked into linear chains in the solid state through interactions with potassium ions. A weak antiferromagnetic coupling, mediated by O–Mo–O exchange pathways, occurred between neighbouring iron centres, resulting in a highly symmetrical geometric frustration despite no changes in the overall architecture.

ENDOEDRAL FULLERENES

Cage within a cage

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There is a broad range of compounds that consist of fullerene cages enclosing various metal atoms — known as endohedral metallofullerenes. They range from C_{60} cages with one or two small atoms inside, to large C_{80} to C_{84} cages containing several metal atoms, such as $\text{Sc}_4\text{O}_2@C_{84}$. A cage with the formula $\text{Sc}_4@C_{82}$ has recently been predicted (*J. Phys. Chem. B* **110**, 11098–11102; 2006) to in fact be a C_{80} cage, with the extra two carbon atoms to be found inside.

Now, Tai-Shan Wang and colleagues from Beijing and Xiamen have confirmed their predictions by synthesizing $\text{Sc}_4\text{C}_2@C_{80}$. They further discovered that the structure

is ‘doubly caged’, with a C_2 dimer inside a Sc_4 tetrahedron that is itself within the C_{80} icosahedron. This ‘Russian doll’ compound was made by the Krächmer–Huffman method, Soxhlet-extracted in toluene and then purified by HPLC.

Carbon-13 NMR spectroscopy confirmed that the fullerene was C_{80} , with only two carbon environments; no C_{82} cage could provide such a spectrum. The metal carbide endofullerene is very stable, with cyclic voltammetry experiments and density functional theory (DFT) calculations suggesting a bandgap of around 1.6 eV. Three bands in the infrared spectrum confirmed the presence of three types of scandium–carbon bonds, confirming the ‘Russian doll’ structure predicted by DFT.

MEDICINAL CHEMISTRY

Target acquired

Nature **462**, 175–181 (2009)

Drug molecules are usually designed to bind to and modulate the action of a specific biological target. That such selectivity is rarely achieved in practice is demonstrated by the various side effects and the efficacy of drugs. Moreover, although some more recently developed drugs may have originally been designed for specificity, they are known to act through multiple targets in a way that is therapeutically essential.

Now, Brian Shoichet from the University of California, San Francisco, Bryan Roth from the University of North Carolina and co-workers have turned this to their advantage. Instead of comparing similarities — such as protein sequence — between targets they have created a map that relates targets by the drugs that bind to them. They took 3,665 known FDA-approved and investigational drugs, and identified several previously unanticipated drug–target associations, including five that were shown experimentally to be potent (with binding constants <100 nm).

The interest in these newly acquired targets is threefold. Firstly, some off-target associations may be the major cause of side-effects that now warrant further investigation and, secondly, others may provide important new opportunities for as yet undiscovered therapeutic intervention. Finally, some of these drugs may exert their effect by acting at a different target to that previously thought and thus improve our knowledge of their mechanism of action.

The definitive versions of these Research Highlights first appeared on the *Nature Chemistry* website, along with other articles that will not appear in print. If citing these articles, please refer to the web version.

blogroll

Goodbye to Kyle

Alas, poor Chem Blog! We knew it, readers: a blog of infinite jest, of most excellent fancy.

In a post entitled ‘The final step in evolution is extinction’ (<http://go.nature.com/TFm593>), Kyle Finchsigmate announced that he has stopped blogging. In his own words “I think I have pushed it far enough and I have reached the end of my intellectual interest and now wish to divest myself from blogging”. Its passing did not go unnoticed and Mitch recorded the event on The Chemistry Blog (<http://go.nature.com/Gj85Nx>). He paid “homage to the great Kyle Finchsigmate’s influential chemical blog...he was able to get away with his potty-mouth antics in a way to be informative, cutting, and always entertaining”. Beyond the antics, Mitch reminds us that it “served as a vehicle to develop his capacity to analyze literature and communicate his insights to the chemical community”.

On a more serious note, a post by Yudhijit Bhattacharjee on the ScienceInsider blog (<http://go.nature.com/bdQAKi>) discussed a recent report challenging the received wisdom that the USA needs more science, technology, engineering or math(s) (STEM) graduates. In a nutshell, the paper presented at the Annual Meetings of the Association for Public Policy Analysis and Management suggests that “US colleges and universities produce three times more STEM graduates every year than the number of STEM jobs available”. This oversupply depresses wages and leads to high-performing students turning away from science. Comments were pretty forthright, with many people bemoaning the low levels of both jobs and remuneration in STEM.

What do you do when your trusty calculator breaks down? The answer, according to Chiral Jones (<http://go.nature.com/TxCTWt>), is to use Google. “In addition [to the answer], it’ll also spit out whatever it interprets as its actual search.” And in many cases, that turns out to geographical coordinates — any more hits in Senegal and Jones will be taking it as a sign to enter the Dakar Rally!