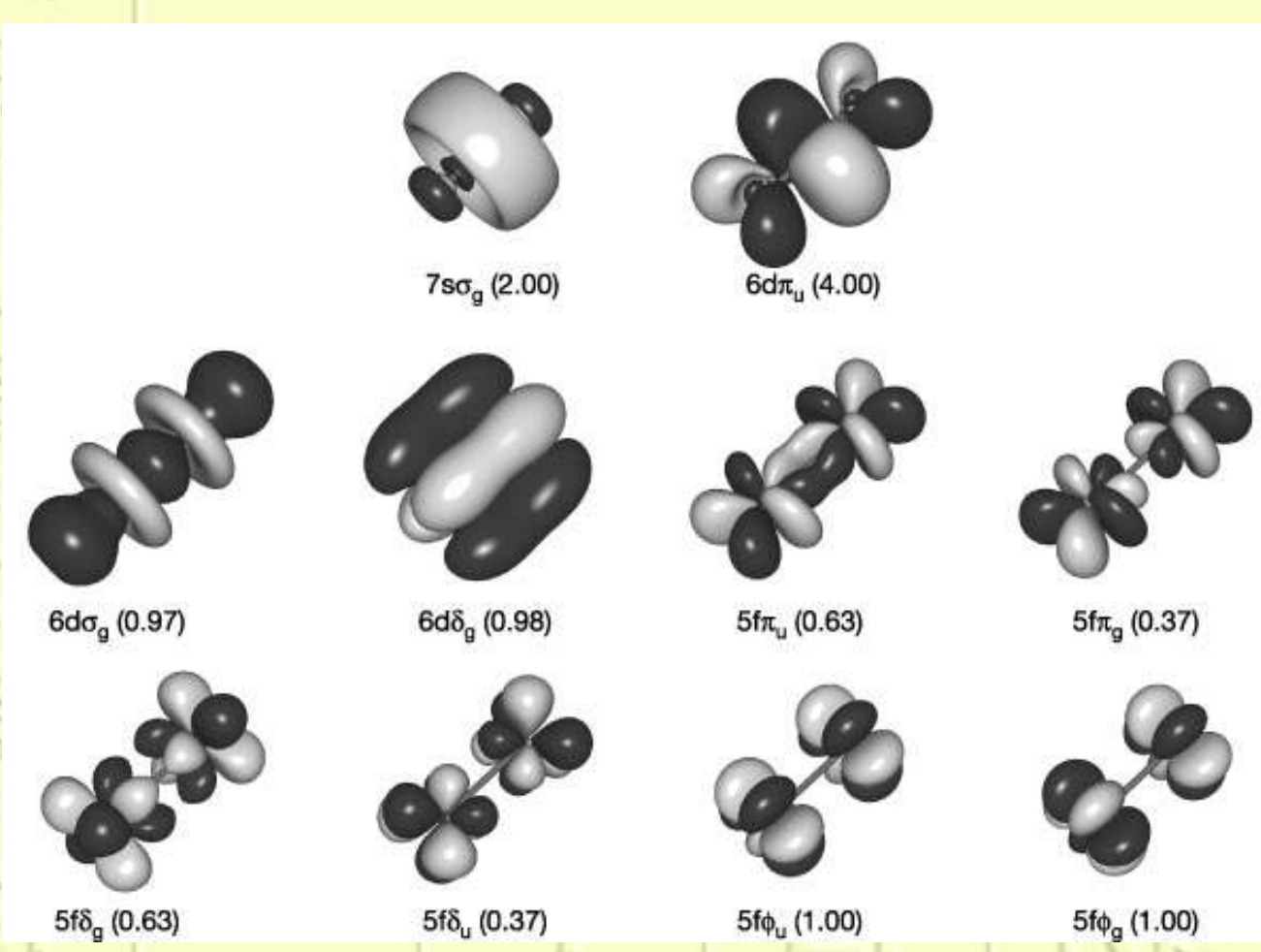


## Enllaços quintuples en la molècula de U<sub>2</sub>

Using advanced quantum chemical calculations, Laura Gagliardi of the University of Palermo, in Italy, and Björn O. Roos of Lund University, in Sweden, find that uranium atoms in diuranium compounds are held together with five covalent bonds--the equivalent of a quintuple bond [*Nature*, **433**, 848 (2005)].

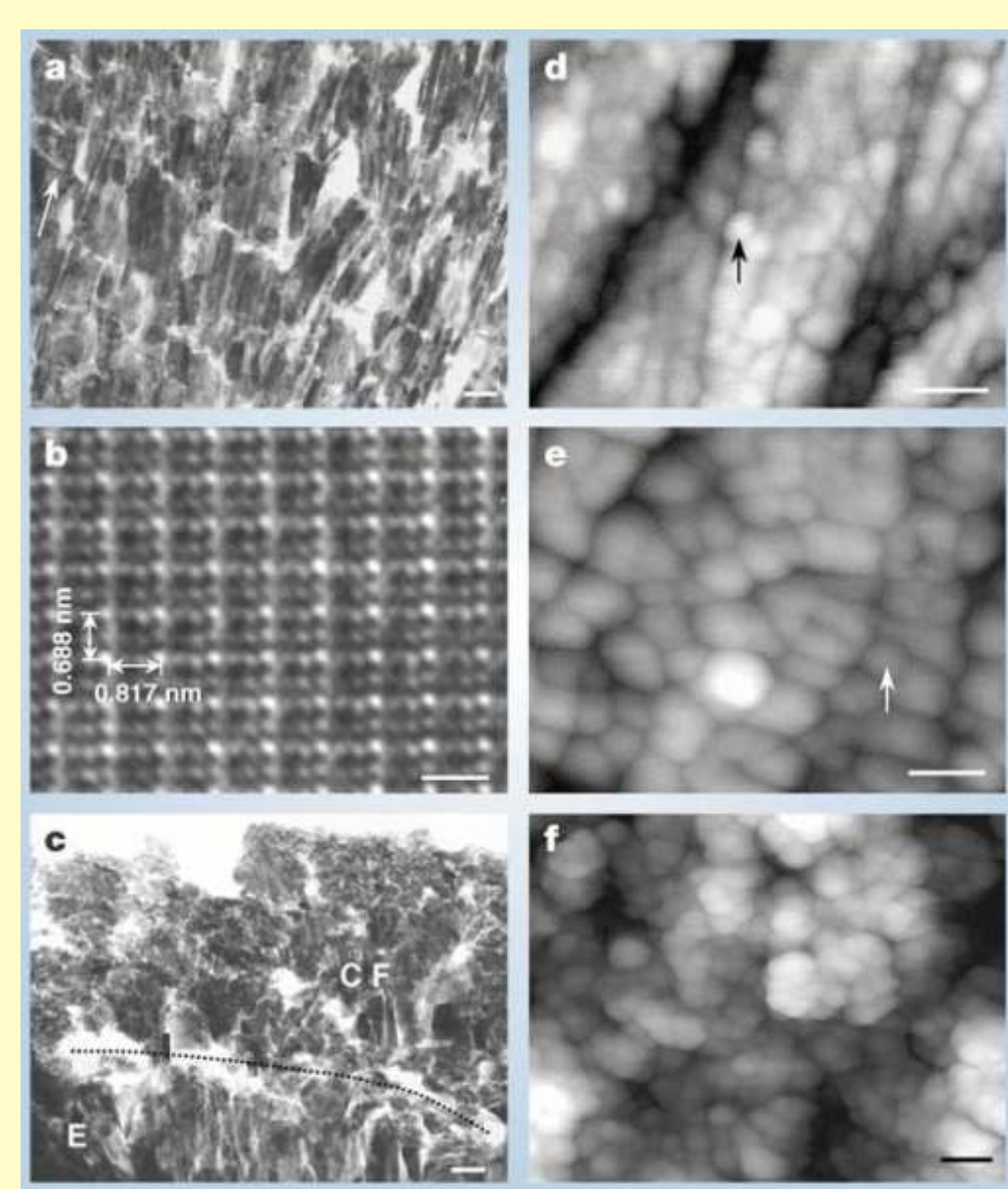
Complex binding is expected when many atomic orbitals and valence electrons are available to participate in bonding. For example, quadruple metal-metal bonds have been observed for transition metals. The new results show that metal-metal multiple bonding involving actinide metals, where f orbitals can participate, is even more complex. The few known diuranium compounds have been observed only spectroscopically, and theoretical studies have been limited. Gagliardi and Roos examined U<sub>2</sub>, where each uranium atom has six valence electrons and 16 atomic orbitals available for bonding. They find that 10 electrons form three traditional two-electron bonds and four single-electron bonds, which translates to a quintuple bond. The two remaining valence electrons are in nonbonding orbitals, one on each uranium atom, and their electron spins couple to provide additional bonding.



## Pasta de dents curativa

Synthetic tooth enamel developed by Japanese researchers could make it easier to repair the tiny lesions in teeth that mark the start of tooth decay [*Nature*, **433**, 819 (2005)]. Because these early cavities are smaller than 50 μm, conventional filling materials tend not to stick to them. Dentists have had to treat them by either removing a large amount of healthy tooth so that the filling sticks or by fortifying the decayed area with fluoride rinse.

Now, Kazuo Yamagishi of Tokyo's FAP Dental Institute and coworkers have prepared a paste that can seamlessly repair the early lesions via nanocrystalline growth without the need for painful drilling. The material is made from hydroxyapatite--the same material that makes up natural tooth enamel--that has been treated with fluoride. The synthetic enamel not only repairs early cavities but also strengthens natural enamel and prevents lesions from recurring.



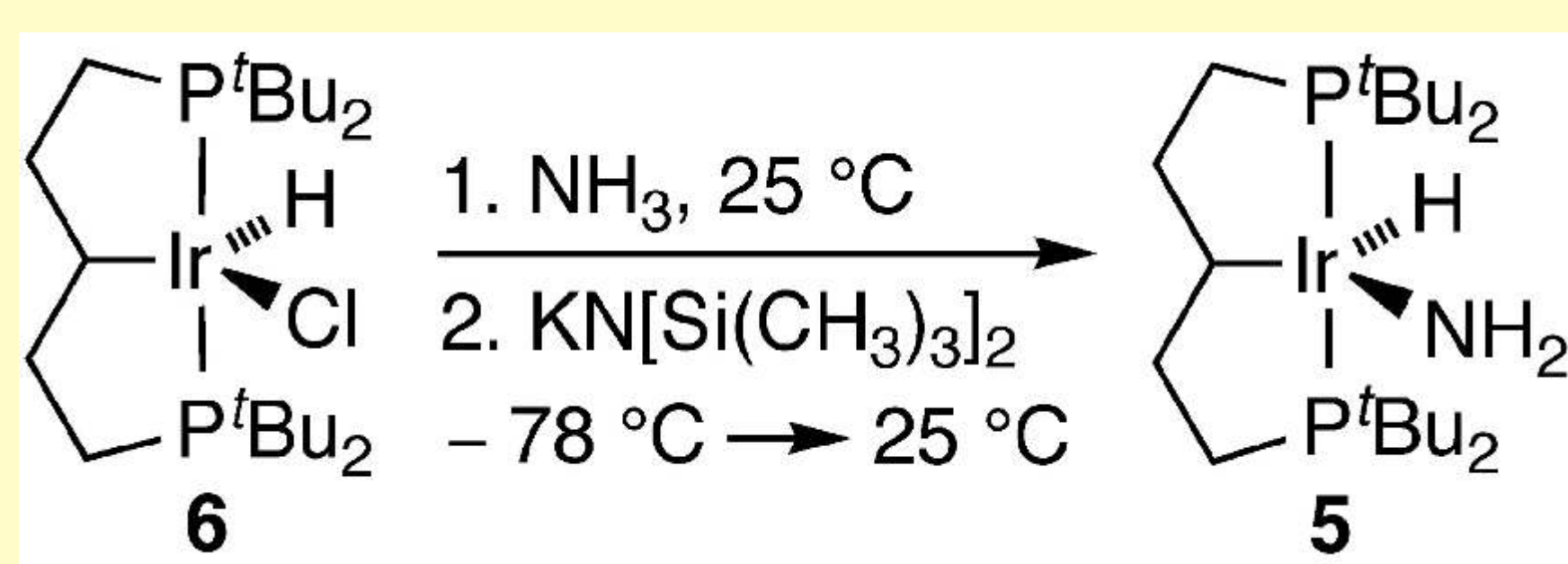
a. Image of the interface between the regrown layer (upper region) and the enamel (lower region); the arrow indicates the direction of the tooth surface. b. Atomic image of a grown crystal of synthetic enamel. c. Tooth treated with acidic phosphate fluoride; dotted line indicates the interface between the calcium fluoride layer (CF) and enamel (E). d. Original enamel surface; arrow, hydroxyapatite crystal. e. Surface after 3 min of repair time; arrow, newly grown hydroxyapatite crystal. f. Surface after completion of repair (15 min). Scale bars: a, c, f, 100 nm; b, 1 nm; d, e, 50 nm.

## L'amoníac, finalment activat

The design and synthesis of an iridium complex that undergoes oxidative addition of ammonia to form an amido hydride derivative appears to have solved one of chemistry's long-standing research challenges: how to activate N-H bonds under mild conditions. This fundamental breakthrough could lead to industrially important catalytic ammonia-transfer processes.

Chemists have known for a century that ammonia forms simple M-NH<sub>3</sub> coordination complexes with most transition metals. Transition-metal complexes also are known to insert into generally unreactive X-H bonds of hydrogen, silanes, boranes, and alkanes (where X = H, Si, B, or C). But no one, until now, had designed a metal-ligand system that is thermodynamically favored to insert into an N-H bond of ammonia.

John F. Hartwig at Yale University and coworkers, have accomplished the feat with an iridium complex that contains a tridentate pincer-type ligand [*Science*, **307**, 1080 (2005)]. The key to their success was increasing the electron density on the already electron-rich iridium atom.

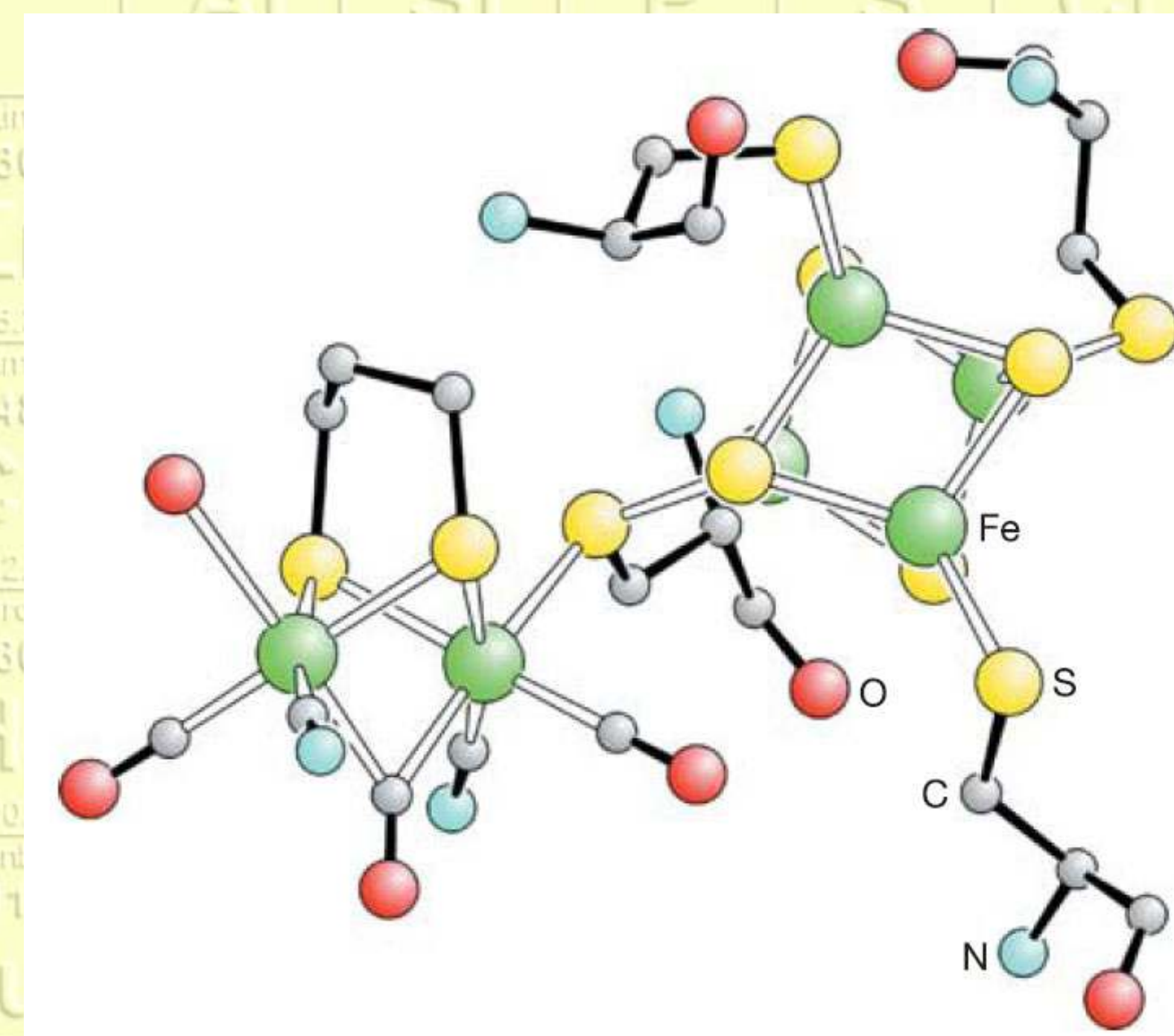


## La hidrogenasa inspira noves cel·les de combustible

The long-sought synthesis of an inorganic complex very similar to the catalytic iron-sulfur core of bacterial hydrogenase suggests that similar synthetic systems could be developed for reversible hydrogen fuel cells that would not require expensive and rare platinum catalysts.

Hydrogenases are enzymes that enable bacteria to evolve or take up hydrogen and use it as a metabolic oxidizing or reducing agent. The new complex accelerates the same reaction as hydrogenase, although less efficiently. It was synthesized by biological chemistry professor Christopher J. Pickett of John Innes Centre, Norwich, England, and collaborators there, at Pacific Northwest National Laboratory, and at the University of Milan-Bicocca, in Italy [*Nature*, **433**, 610 (2005)].

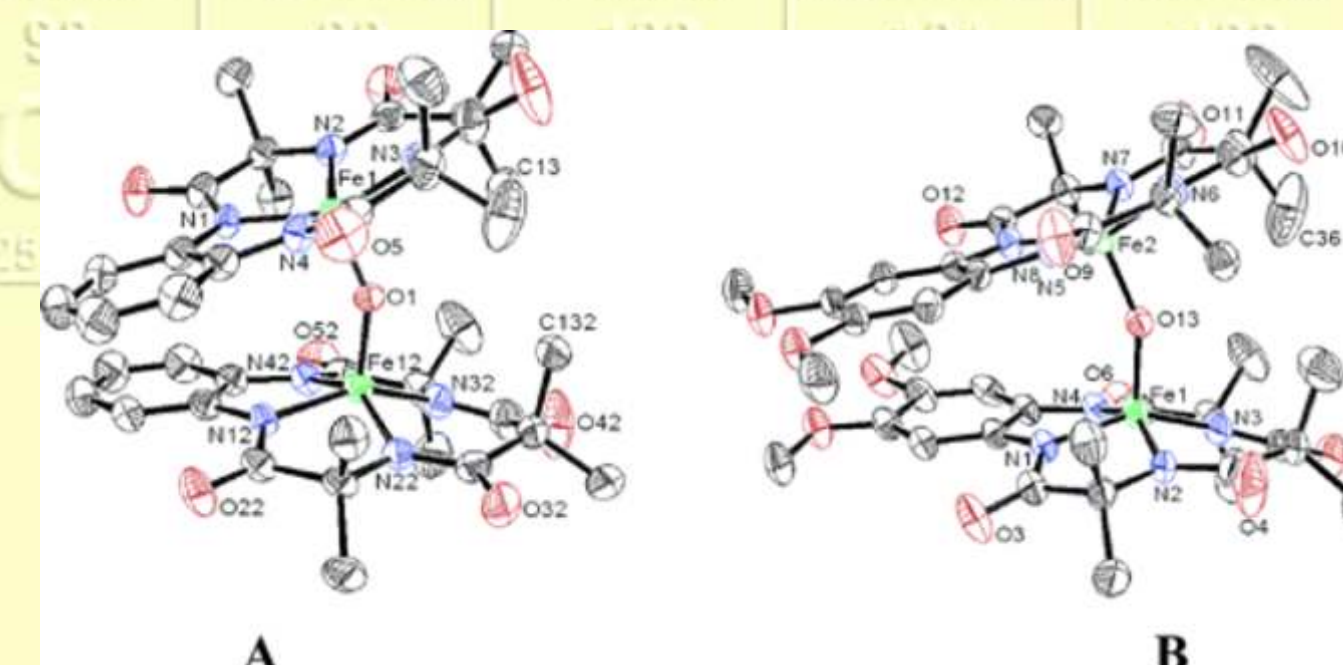
In hydrogenase, the core (H-cluster) consists of two components-- an Fe-Fe unit and a larger 4Fe4S cluster--that are joined through a sulfur atom on one of the enzyme's cysteine residues. The synthesis involved the creation and joining of the two components, which is very difficult. The researchers then showed that the synthetic cluster catalyzes reduction of H<sup>+</sup> to H<sub>2</sub>--currently with poor efficiency, but they hope this can eventually be improved.



## El Fe(IV) més a l'abast

Iron(III) tetraamido macrocyclic ligand (TAML) complexes developed by Carnegie Mellon University chemistry professor Terry Collins increase the oxidizing power of hydrogen peroxide under mild conditions, making the catalysts useful as substitutes for environmentally unfriendly chlorine- and metal-based industrial oxidations. An international team led by Collins has now shown that TAML complexes can facilitate oxidations using molecular oxygen, a process the researchers knew was possible but for which they did not have definitive proof [*J. Am. Chem. Soc.*, **127**, 2505 (2005)].

Previously, only iron(II) complexes were known to react this way with O<sub>2</sub>. The team reacted solutions of a TAML complex (shown) with O<sub>2</sub> at room temperature to generate an iron(IV) TAML dimer in which the iron atoms are linked by a bridging oxygen atom abstracted from O<sub>2</sub>. The dimer catalytically oxidizes alcohols to aldehydes and phosphines to phosphine oxides. The initial TAML complex is regenerated in the process. This new type of iron-oxygen chemistry is important in understanding biological oxidation processes and could further improve industrial oxidations



## Breus

- La Societat Catalana de Química ha iniciat la publicació de la col·lecció *Clàssics de la Química*, en la que es traduiran al català els treballs més importants de la Química. El primer número correspon a "L'atom i la molècula" de G.N. Lewis, aparegut a *J. Am. Chem. Soc.*, **38**, 762 (1916).
- El Chemical Abstracts recull també les "publicacions més intrigants", segons el judici dels seus experts (<http://www.cas.org/spotlight/scientists.html>).
- S'ha comprovat que els perclorats són molt més habituals al medi ambient del que es pensava [*Chem. Eng. News*, 14 feb. 2005, 10; 7 mar. 2005, 43].
- S'han preparat uns nous purificadors d'aigua, basats en resines d'intercanvi iònic, que es regeneren només escalfant-los [L.J.P. van der Broeke et al., *J. Am. Chem. Soc.*, **127**, 1594 (2005)].

L'element número 21, **escandi**, va ser descobert el 1879 per Lars Fredrik Nilson. El seu nom prové del mot llatí *Scandia*, que significa *Escandinàvia*. Correspon a l'element *ekabor* predit per Mendelejev.