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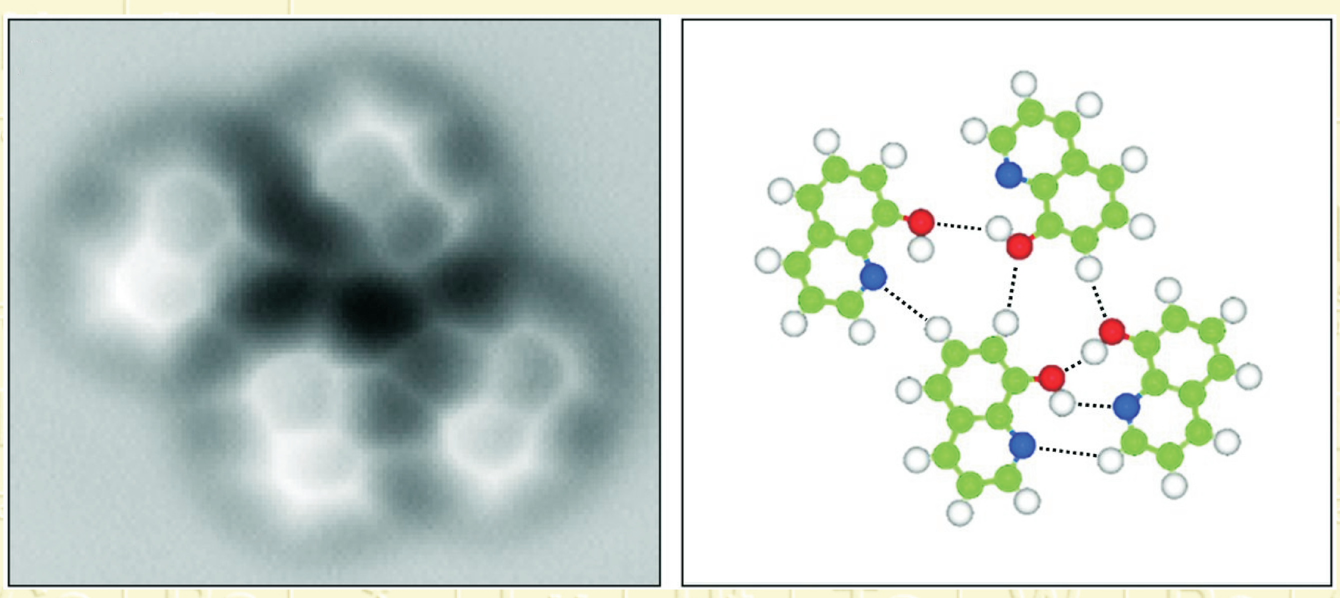
L'enllaç d'hidrogen atrapat

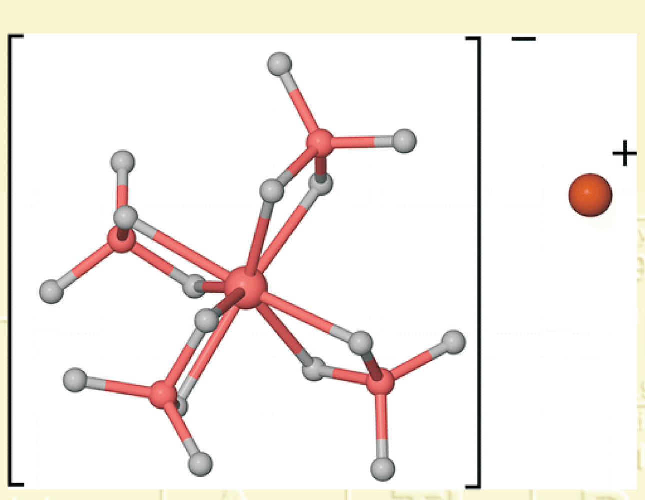
Hydrogen bonds are ubiquitous—and universally important—in chemistry. They give water its unique properties, speed or slow reactions, and hold together the three-dimensional shapes of DNA, proteins, and other supramolecular structures. But chemists have never actually seen them. Now, with high-resolution atomic force microscopy (AFM), they have (J. Zhang et al., *Science,* **2013**, *342*, 611. DOI: 10.1126/science.1242603). The stunning images should enhance understanding of hydrogen bonds' hitherto elusive properties. Using a technique called noncontact AFM to look for intermolecular forces between a variety of compounds, the authors succeeded with 8-hydroxyquinoline deposited on a copper surface. At temperatures near absolute zero, they found that 8-hydroxyquinoline formed hydrogen-bonded aggregates, with the electron density of the hydrogen bonds made visible by AFM. At room temperature, the researchers also observed hydrogen bonds in dimers and trimers of 8-hydroxyquinoline radicals complexed with copper. The species likely formed through a previously known dehydrogenation reaction of hydroxyl groups on copper surfaces.



AFM images of 8-hydroxyquinoline on a copper surface shown hydrogen bonding intercations at room temperature. C=green; H=white; O=red; N=blue; Cu=orange

L'electronegativitat no té límit

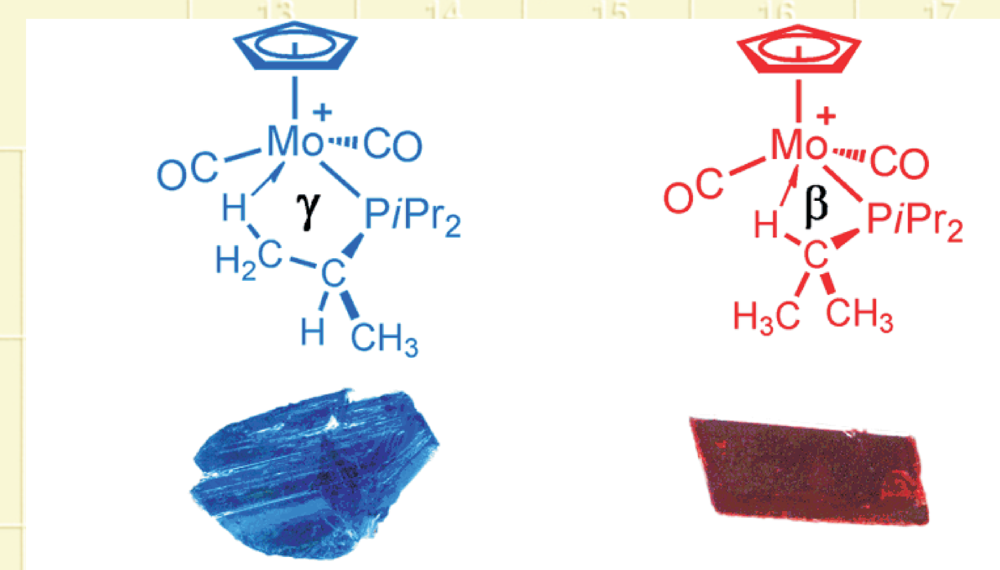
A few years ago, it was discovered a class of compounds with unprecedented electronegativities called hyperhalogens. These compounds are made of a metal atom surrounded by superhalogens—which themselves are highly electronegative molecules made of a central atom surrounded by an electronegative element or group. Hyperhalogens hold promise as superoxidizers that could be used as a rocket fuel or as hydrogen storage materials if they can be tamed into a stable form. Now (D. A. Knight, et al., *J. Phys. Chem. C,* **2013**, *117*, 19905. DOI: 10.1021/jp407230a) it has been synthesized and characterized a stable hyperhalogen salt, $K[Al(BH_4)_4]$, whose anion, $Al(BH_4)_4^-$, has an extremely high electron affinity They prepared the compound by coupling $Al(BH_4)_3$ with KBH_4. Unlike the few hypersalts synthesized so far, this new salt is stable at temperatures of up to 154 °C. Besides providing a new functional material, the work validates the use of computational studies for rational design of new compounds based on superhalogens and hyperhalogens.



Estructura del $K[Al(BH_4)_4]$

Isomerització a tot color

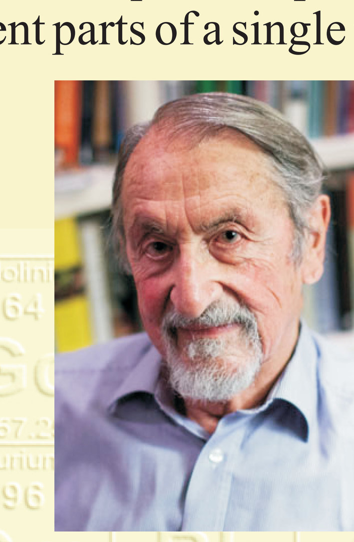
The appearance of two types of crystals—some red, some blue—in a reaction vessel thought to contain a single product might spell trouble; impurities, for example. But an observation of that type, has instead deepened understanding of isomerization in complexes with agostic bonds. An agostic bond is a type of bonding between a transition-metal atom (M) and a C–H unit that involves a threecenter, two-electron arrangement (C–H–M). The bond stabilizes some organometallic complexes, including ones at the center of homogeneous catalytic processes. Researchers have known for years that some agostic complexes undergo rapid interconversion in solution between structurally isomeric forms, each of which retains the original agostic bond. Now it has been reported that isomerization can unexpectedly cause an agostic molybdenum phosphine complex to crystallize in two forms (E. F. van der Eide, et al., *Angew. Chem. Int. Ed.*, **2013**, *52*, 10190. DOI: 10.1002/anie.201305032). Each isomer has a distinct molecular orbital configuration and hence a distinct color.



Nobel per als fonaments computacionals

The 2013 Nobel prize in chemistry has been awarded to Martin Karplus of Harvard University, Michael Levitt of Stanford University, and Arieh Warshel of the University of Southern California, for 'the development of multi-scale models for complex chemical systems'. Their work in the 1970s led to the development of fundamental computational tools that are used today to model complex chemical reactions, such as the split-second molecular changes occurring during photosynthesis, or within enzymes and receptors in the body. One of the trio's landmark contributions to the field was finding a way to combine quantum physics with classical physics to model the interactions between different atoms and molecules.

The quantum theoretical calculations needed to simulate chemical reactions require a huge amount of computational power. Calculating how atoms and molecules interact using classical physics is comparatively simple by contrast and can be used to model much larger molecules, but cannot be used to calculate the behaviour of atoms during reactions. Chemists once had to base their models on one or the other, but Karplus, Levitt and Warshel developed computer models that could apply quantum and classical calculations to different parts of a single molecule.



Martin Karplus

Michael Levitt

Arieh Warshel

Breus

• Aquest any i com a conseqüència de la nova definició del kilo, vegeu ***Notícies Inorgàniques*, 58**, febrer 2012, la IUPAC ha decidit revisar el pes atòmic de 19 elements: Be, F, Al, P, Sc, Mn, Co, As, Se, Y, Nb, Mo, Cd, Cs, Pr, Ho, Tm, Au, Th.

• El departament de publicacions de l' American Chemical Society, ha implantat el servei anomenat **CrossCheck**, per tal d'evitar plagis en els articles publicats en les seves revistes.

• La Societat Alemanya de Química ha elaborat un informe crític, de més de 700 pàgines, sobre la seva actuació durant el període del nazisme. El conglomerat d'indústries químiques IG Farben que incloïa BASF, Bayer, Agfa i Hoechst col·laborà de manera clara i eficaç amb els mètodes d'extermini aplicats en els camps de concentració. Al número de 30 de setembre de *Chem. Eng. News*, **2013**, *91(37),* 30, s'hi pot trobar un resum ampli.

Avui recomanem

La desena exposició de la tradicional Mostra del Fons Històric de la Biblioteca de Física i Química, dedicada enguany a commemorar el centenari del popular model atòmic proposat per Niels Bohr (1885-1962). **«L'Àtom de Bohr. 100 anys en òrbita»** es podrà veure durant tot el curs 2013-2014.

L'element

L'element número 65, **terbi**, fou descobert pel químic suec Carl Gustaf Mosander l'any 1843 que el detectà com a una impuresa en la itèrbia, l'òxid d'itri, Y_2O_3; el nom prové del del poble suec Ytterby; no fou aïllat, però, fins l'any 1905 aplicant els nous mètodes d'intercanvi iònic.

Té un aspecte com la plata, és prou tou per poder-se tallar amb un ganivet i bastant estable a l'aire, si bé s'oxida lentament i reacciona amb l'aigua.

A l'igual que els altres lantànids els compostos de terbi tenen una toxicitat moderada, encara que no ha estat gaire estudiada i no se li coneix cap activitat biològica.

No té gaires aplicacions pràctiques perquè és un element poc abundant i difícil d'obtenir. La producció anual és de l'ordre de 10 Tm anuals i és quatre vegades més car que el platí.

Una propietat poc habitual és que els aliatges que el contenen, com el $Tb_{0.3}Dy_{0.5}Fe$, s'allarguen o escurcen en presència d'un camp magnètic, fet que permet emmagatzemar energia de tensió i que actualment és estudiada per tal d' aprofitar-la en motors, bombes o sistemes d'injecció. Alguns fòsfors que el contenen són útils en medicina en augmentar la seguretat de les exploracions amb raigs X, ja que redueixen sensiblement els temps d'exposició necessari dels pacients.