



Máster en Química Avanzada. Preparación y Caracterización de Materiales.

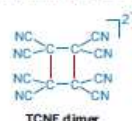
Organiza: Departamento de Química Física

CONFERENCIA:

Exploiting benzene's unknown Mr Hyde character to develop new photochemistry

UNIQUE MULTICENTER BOND CONFIRMED

Chemical bonds typically involve two atoms sharing one or more pairs of electrons. But chemists keep finding molecules that defy that norm. For example, some electron-deficient molecules exhibit multicenter bonding with three atoms sharing two electrons. A dozen years ago, Joel S. Miller of the University of Utah and his colleagues discovered an unusual type of multicenter bonding: a molecule with a four-atom, two-electron bond. Miller's team came across the anomaly when preparing magnetic materials from transition-metal complexes that include the radical anion tetracyanoethylene (TCNE). In the crystal structures they found that two TCNE units form a dimer (shown) in which the central carbons are separated by 2.9 Å. That distance exceeds conventional C–C bond lengths, which are in the range of 1.5 Å, but it is still close enough to suggest a bonding interaction. In addition, the dimer's structural, spectroscopic, and magnetic properties point to a four-carbon, two-electron bond that is stronger than hydrogen bonds. "But there has still been a concern whether the bond really exists," Miller says. His team now has definitive proof after elucidating telltale vibrational flexing of the bond by Raman spectroscopy (*Angew. Chem. Int. Ed.*, DOI: 10.1002/anie.201207813). Better understanding of this unique bonding could ultimately lead to new molecules with interesting magnetic and other properties, Miller notes. —SR



TCNE dimer

This tetracyanoethylene dimer is held together by a two-electron bond (red lines) between four carbon atoms.

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Molecule of the Week

Tetracyanoethylene

Tetracyanoethylene (TCNE) is a crystalline solid with a melting point of 205 °C. Quinone derivatives produced in 1932 by reaction of tetracyanoethylene with isobutene in boiling benzene. TCNE is an excellent electron acceptor and has been used to prepare organic superconductors.

In 2011, J. S. Miller and co-workers at the University of Utah (Utah State Chem) discovered that the TCNE radical anion forms a dimeric dimer. They believed that the dimer contains an unusual four-atom, two-electron bond that connects the four radical carbon atoms. Recently, Miller and colleagues used Raman spectroscopy to confirm the existence of the four-carbon bond.

More about this molecule from CAS, the most authoritative and comprehensive source for chemical information.

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Viernes 9 de octubre 2014

Aula: M2, Louis Lions

Hora: 12.00 h