



Máster en Química Avanzada. Preparación y Caracterización de Materiales.

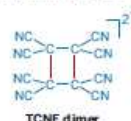
Organiza: Departamento de Química Física

## 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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Viernes 9 de octubre 2014  
Aula: M2, Louis Lions  
Hora: 12.00 h