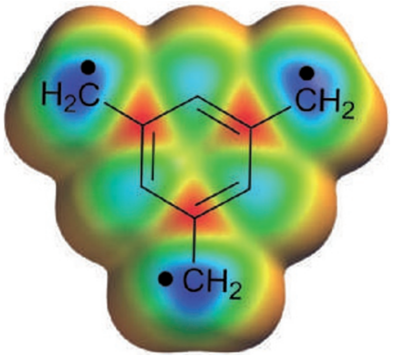
or sulfonylation in a straightforward fashion from either a sulfonamide or an arylamine respectively. Thus, when combined with the large number of strategies known for N-arylation and N-sulfonylation of amines, the synthesis of the necessary leaving group is easily achievable. Reactions with stereodefined amines show that the substitution occurs with inversion, that is by an S_N2 mechanism, and Urabe and co-workers describe substitutions with nitrogen, oxygen and carbon nucleophiles.

At present, only intramolecular reactions have been carried out, and the reaction conditions (base, 150 °C in DMF) are relatively harsh. These limitations, however, are sure to be the subject of future research efforts along with synthetic applications of the methodology.

HIGH-SPIN ORGANICS

Trapped triradical

Angew. Chem. Int. Ed. **40,** 7277–7280 (2010)



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In the quest for organic magnetic materials, attention has focused on preparing high-spin polyradicals, in particular by using moieties that enable intramolecular ferromagnetic coupling between free radicals. But even though triradical trimethylenebenzene has provided the framework for several such high-spin compounds, it has so far eluded characterization. Patrik Neuhaus and Wolfram Sander from the Ruhr University in Bochum, Germany, have now succeeded in isolating and characterizing it in an argon matrix.

The precursor *tris*(iodomethyl)benzene was subjected to flash vacuum pyrolysis at 480 °C. The products were subsequently isolated in an argon matrix, and characterized through infrared, UV–visible and electron paramagnetic resonance spectroscopy. These measurements revealed that the main product was a highly symmetrical triradical compound that possesses a quartet ground state, a description that fits the elusive trimethylenebenzene well. Derivatives bearing either one or two methyl groups rather than methylene radicals were also found to be present, but only as minor by-products.

The identity of the triradical was further supported by experiments carried out with deuterated methylene groups. It is also in good agreement with previous theoretical studies, which had shown that the triradical should possess both doublet and quartet spin states. Furthermore, in contrast to the widely used *meta*-dimethylenebenzene unit, the trimethylene derivative proved to be relatively stable to UV irradiation — an attractive property for the construction of magnets.

PROTON TRANSFER

Water discovery

J. Am. Chem. Soc. **132,** 11395–11397 (2010)

The way by which protons travel through bulk water has been debated for years, with the concept of structural (or 'Grotthuss') diffusion forming the cornerstone of such discussions. The mechanism is different from that of conventional mass diffusion — whereby a specific atom or molecule randomly moves through a medium — and instead involves the hopping of an excess proton between water molecules through bond formation and cleavage. The process is thought to occur through the interconversion of Eigen $[H_3O^+(H_2O)_3]$ and Zundel $[H_2O\cdots H\cdots OH_2]^+$ complexes.

Recently, attention has turned to the mechanism of proton transport in confined spaces, and now a team led by Gregory Voth of the University of Chicago and Tianying Yan of Nankai University have studied theoretically how protons travel along a one-dimensional chain of water molecules within a narrow carbon nanotube. Simulating the system is beyond the scope of traditional molecular dynamics methods and they therefore use multistate empirical valence bond molecular dynamics that can better describe the bond breaking and formation involved in proton transport.

They calculate the probability distribution of the distance between the oxygen atoms of adjacent water molecules and the displacement of the charge that results from the excess proton. The calculations reveal that the proton is usually hydrated as part of a distorted Zundel cation, and that proton transfer within a narrow carbon nanotube occurs through a Zundel-to-Zundel mechanism. This behaviour differs from that observed in bulk water, and can be attributed to the reduced dimensions of the system.

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 original web version.

blogroll

Different in theory

Comparing physics with chemistry, and theory with experiment — and a boost for chemistry

The Curious Wavefunction blog discusses 'The difference between chemistry and physics' (http://go.nature.com/vcWIdr) kicking off with a quote from William Lipscomb: "Chemistry is not 'physics with less rigor'. In chemistry there are discoverable guiding principles for systems which are too complex for a 'first principles' approach. The nature of chemistry is very difficult to explain to most physicists, in my experience!" Wavefunction agrees, saying "One has to think at the level of molecules and not just atoms [...] Knowing about quarks won't directly help you to understand the structure of DNA but knowing about hydrogen bonds definitely will."

Derek Lowe is similarly philosophical at In the Pipeline (http://go.nature.com/FIKJTQ), discussing the relative value of theory and experiment. He contrasts the fame of theoretical physicists like Einstein, Feynmann and Hawking with the fact that "Chemistry [...] has always been an experimental science in the public mind. Say 'chemist', and people think of someone in a lab coat, in a lab, surrounded by chemicals." But that's not a bad thing according to Lowe, because experiments are crucial in any field of science, and chemistry will always have enough experiments to go around.

We often grumble about the lack of credit chemists get in the wider public, so we're glad to see Eric Drexler addressing the balance (http://go.nature.com/Sp6Bca). He picks up on an article (http://go.nature.com/ZREgHV) about the 150th anniversary of what C&EN calls 'the first-ever international scientific conference', back in 1860 in Karlsruhe. The conference — suggested by Kekulé — was attended by some of ninteenth-century-chemistry's greatest names: Bunsen, Mendeleev and Erlenmeyer. The aim was to cut through the confusion and dissent among the international community about the composition of molecules. Although the conference didn't lead to immediate sweetness and light, the seeds were sown for the acceptance of Avogadro's perspective.