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Spotlights on Recent *JACS* Publications

HIGH-SPIN ORGANIC POLYRADICALS BEAT THE HEAT

Andrzej Rajca and co-workers have successfully synthesized a new series of organic magnetic materials with improved stability (DOI: 10.1021/ja409472f). These materials have potential application in a wide variety of areas including metal-free and more biologically friendly contrast agents for magnetic resonance imaging. Typically, such materials have suffered from being very short-lived species, stable only at impractically low temperatures.

The researchers have designed, synthesized, and magnetically characterized aminyl tetraradical structures, which are π-conjugated organic polyradicals with a high-spin ground state. The high-spin ground state gives these molecules unusually strong paramagnetic properties, similar to those typically found in metal-containing molecules. The chemists include key design elements into the structure to achieve the desired magnetic performance and show that, at temperatures up to 100 K, these radicals are stable and are found exclusively in the high-spin ground state. This work demonstrates the rational design of a complex molecule, coupled with its synthesis. This type of process could be applied to design materials targeting specific performance attributes for practical applications.

Dalia Yablon, Ph.D.

HIGH-TEMPERATURE INSULATOR HAS METALLIC POTENTIAL

Boron nitride (BN) is a classic insulating material. Stable and heat resistant, BN is commonly used in high-temperature components, lubricants, and electronic insulators. With boron just to the left of carbon in the periodic table, and nitrogen just to the right, many properties of BN mirror those of its better-known neighbor.

Recently, BN has attracted the interest of the nanotech community because, like carbon nanotubes, BN atoms will line up in a hexagonal sheet and curl into a tiny tube. Unlike carbon, BN remains an insulator, no matter how much it is rolled or squeezed, or what pattern its atoms arrange themselves into—at least, that is what researchers used to think.

Now Qian Wang and co-workers show that BN can become conductive without atomic additives and still maintain its prized stability (DOI: 10.1021/ja410088y). The researchers describe a theoretical form of BN in which tetragonal atomic arrangements work together to free electrons for conduction. The authors note that a metallic form of BN could benefit applications that include electron transport, metal-free catalysis, and harsh-environment electronic devices, and they hope that their theoretical discovery will spur experimentalists to create the first intrinsically conductive BN.

Jenny Morber, Ph.D.

MOLECULAR CAPSULES EXHIBIT EXOTIC PROPERTIES IN WATER

Julius Rebek and co-workers demonstrate a new type of water-stable hydrogen-bonded capsule that broadens the range of small-molecule payloads at neutral pH and represents a new venue for exploring molecular behavior in small places (DOI: 10.1021/ja410644p).

Molecules in solution behave very differently when confined to small spaces, such as inside nanosized capsules. Instead of randomly encountering other molecules in bulk solution, they experience prolonged and intensified interactions with each other at close range. Confinement can also amplify stereochemical effects and provide a stable environment for otherwise reactive species. Molecular containers known as hydrogen-bonded capsules are made of molecules that self-assemble on the basis of hydrogen bonding, metal–ligand interactions, and hydrophobic effects. Since water competes with the forces that drive their assembly, water-compatible hydrogen-bonded capsules have been an enormous challenge to create.

The team introduces hydrophobic groups in key positions on a well-studied class of capsule building blocks, known as a benzimidazolone cavitands. The new cavitand derivatives dimerize in water to form capsules capable of trapping hydrophobic "guest" molecules inside. Since the vessel interior is hydrophobic, the molecular interactions between the cavitands and guest molecules are not disrupted by water.

Christine Herman, Ph.D.

LONG LIVE METHYL FOR BOOSTING MRI SIGNALS

Magnetic resonance imaging (MRI) creates detailed images of the inner workings of the human body, aiding in the study and treatment of diseases. The strength of MRI signals, though, is limited, in part, because most molecules have short-lived nuclear spin states. Scientists are working on strategies to increase signal strength, which may help improve visualization of physiological features such as tumors. One approach utilizes molecules with long-lived spin states that increase MRI signal strength via a phenomenon called hyperpolarization. The problem is that only molecules with a very specific type of structural symmetry can achieve such long-lived states, limiting the technique's potential in MRI.

A new study suggests there may be more opportunities than previously believed for the generation of long-lived spin states. Malcolm Levitt and colleagues find that rapidly rotating methyl groups, which are found in a wide range of biological molecules, can achieve a long-lived state (DOI: 10.1021/ja410432f). This finding could greatly increase the number of molecules that are capable of enhancing signal intensity in MRI. The study also explains a previous observation of strong signal enhancements for ^{13}C-γ-picoline, which contains a rapidly rotating methyl group.

Erika Gebel Berg, Ph.D.

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