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Spotlights on Recent *JACS* Publications

CLOSING THE LOOP ON A PATHOGEN'S STRATEGY

Linda Columbus and colleagues report the structure and dynamics of an outer membrane protein that the bacteria that cause gonorrhea and meningococcal meningitis—two different species of *Neisseria*—use to invade host cells (DOI: 10.1021/ja503093y). Gonorrhea and meningococcal meningitis are caused by two different species of Gram-negative bacteria.

When certain outer membrane proteins of these bacteria bind to receptors on the surface of a host cell, they induce phagocytosis, allowing the bacteria to enter the cell. These bacterial membrane proteins have several extracellular loops with high sequence diversity that helps them evade the host's immune system. Scientists want to understand how these proteins can bind a common set of receptors despite the high variability of their loops.

Using NMR and molecular dynamics simulations, Columbus and co-workers find that the protein's three extracellular loops are extremely dynamic, shifting conformation on a time scale of nanoseconds. They propose that the plasticity of these regions allows them to engage a common set of receptors despite their high sequence diversity. The work illuminates how pathogenic bacteria balance evading and invading their hosts. Notably, understanding the structure and dynamics of these proteins could also help researchers design similar proteins to deliver drugs to cells.

Deirdre Lockwood, Ph.D.

IMPROVED X-RAY METHOD TO PROBE METAL–LIGAND INTERACTIONS

Serena DeBeer and co-workers describe an improved method of X-ray absorption spectroscopy (XAS) that detects fluorescence from valence-to-core (Vtc) X-ray emission features and can selectively provide specific information on metal–ligand interactions (DOI: 10.1021/ja504206y).

Classic XAS is widely used in inorganic chemistry to characterize the environment around metals. This technique can provide information about the geometry and electronic structures of transition metal complexes, but because only the average of all of the metal–ligand interactions present is detected, details regarding specific metal–ligand interactions remain elusive.

By monitoring fluorescence from Vtc-detected X-ray emission events and then combining it with X-ray absorption, the authors develop a method that extracts significantly more chemical information than either method used alone and offers the possibility of ligand differentiation. They demonstrate the utility of this method by conducting VtC XAS experiments on well-defined manganese complexes that show dramatic spectral changes influenced by ligand identity and electronic structure.

Spectroscopic methods with such selectivity toward ligands are highly desirable when probing small-molecule organometallic or bioinorganic catalysts, where the interaction between a metal center and its substrate or an intermediate might be of primary interest.

Dalia Yablon, Ph.D.

ISOLATION OF A NEVER-BEFORE-SEEN BIRADICAL

Theoretical models from more than a decade ago predicted the existence of disilicon tetrachloride (Si_2Cl_4). But the molecule, which was believed to be an intermediate in the dechlorination of silicon tetrachloride ($SiCl_4$), has never been experimentally synthesized and isolated—until now.

Researchers led by Debasis Koley and Herbert Roesky report the isolation of a singlet biradical form of Si_2Cl_4 (DOI: 10.1021/ja505817u). The precursors $SiCl_3$ or $SiCl_4$ are reduced using the potassium graphite compound KC_8 at low temperature to form dark green crystals of Si_2Cl_4. The molecule can be stored at room temperature under an inert atmosphere when stabilized with two molecules of cyclic alkyl(amino) carbene.

The team has determined the single-crystal structure with synchrotron radiation at 20K, and also uses theoretical calculations to study the electronic structure and bonding of the unprecedented biradical species, which reveal characteristics similar to those predicted previously for the hypothetical Si_2Cl_4 molecule. The compound represents a new member of the polysilicon chloride family, members of which are well-known for their widespread utility in the semiconductor industry and other commercial applications.

Christine Herman, Ph.D.

POLYSACCHARIDE MIMIC KEEPS PROTEINS PERKY

Mark Grinstaff and colleagues have synthesized a novel polysaccharide that mimics natural carbohydrates and is an effective agent for stabilizing proteins for storage (DOI: 10.1021/ja5036804).

Polysaccharides are promising molecules with many biomedical applications, including drug delivery and tissue engineering. But purifying these polymers from biological samples can be problematic: the structure and composition of their monomers can vary, and they can be contaminated by other biomolecules. As a result, scientists seek to control these attributes by synthesizing uniform polysaccharide-like compounds.

Grinstaff and co-workers have found a way to synthesize a polymer with many characteristics of natural polysaccharides, but with a controllable monomeric structure. These poly-amido-saccharides (PASs) are made of glucose-based monomers with an amide linkage. The team also uses a catalyst to make oxidized forms of the polymers.

The PASs can be used to keep proteins from denaturing before they are dehydrated or frozen for storage. An oxidized form of a PAS is shown to be significantly better at stabilizing the protein lysozyme than trehalose, a disaccharide that is commonly used for this purpose. The team's synthetic approach could also help advance the production of other tailor-made polysaccharides for biomedical uses.

Deirdre Lockwood, Ph.D.

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