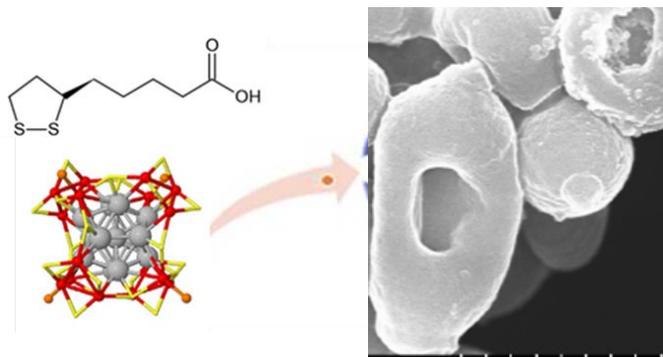


Antiviral & Bactericidal Activity of Silver Lipoate Clusters



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Collaborators:

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Background:

When the surface of a nanometer-scaled noble metal is protected with a suitable ligand, the resulting passivated cluster acquires remarkable physico-chemical stability¹ reminiscent of closed shell atoms. The electronic structure of the emerging super-atom complexes may be described with a simple electron counting model² that guides the quest for stable magic sized structures and the exploitation of their properties in material and biological sciences³

A water soluble super-atom complex of 29 silver atoms and 12 lipoate ligands was recently reported to exhibit promising antibiotic activity⁴ and luminescent behavior.⁵ A standing challenge preventing the exploitation of these intriguing properties is the propensity of the cluster to degrade with time especially when exposed to light and oxygen.⁵ Previous researchers found that the cluster can be regenerated by adding excess reducing agent.⁵

Unpublished Electro spray mass spectrometric analysis by UTSA

collaborators has shown that cluster degradation is accompanied by the

formation of dimers, trimers, etc. suggesting a 2emolytic cleavage of the disulfide bonds of the stabilizing lipoate ligand followed by intercluster disulfide bridging.

A non aqueous homolog of similar silver-lipoate composition has been shown by x-ray diffraction to pose a virus-like icosahedral inner structure (populated by silver atoms enclosed in a

tetrahedral pyramid defined by silver-lipoate ligands ⁶ (Figure 1)

DFT calculations at UTSA predict that the cluster needs four “weakly” coordinating ligands for the structure to converge to that of Bakr et. al.⁶ The minimalist DFT model replaces 12 lipoate ligands with 24 isoelectronic Cl and four PH₃’surrogates for the coordinating ligands. When four waters are used instead of four PH₃’s the structure does not converge. Both structures are compared in Figure 1.

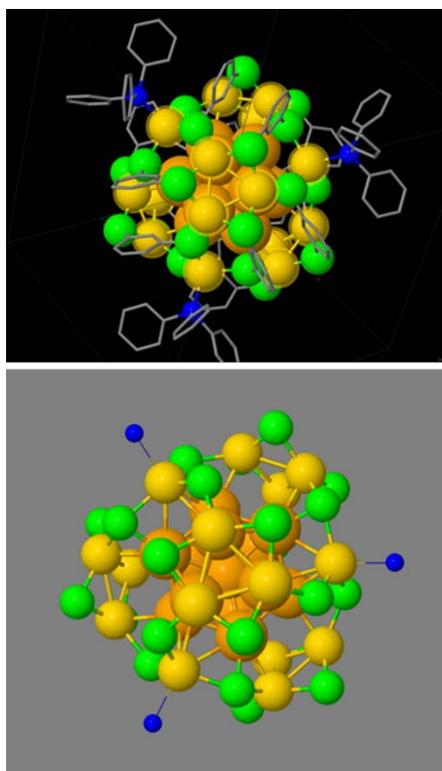


Figure 1: The experimentally determined structure of a Ag₂₉ (top) is predicted theoretically to be attained by the biologically relevant aqueous homolog provided that four weakling coordinating ligands are present.

Goals:

In the Directed Studies chemistry courses at LACC, students will pursue the following objectives:

1. Stabilization of the cluster by storing it under inert conditions. The cluster can be regenerated by purging with nitrogen (unpublished results) or adding excess reducing agent.
2. Stabilize the cluster using weakly coordinating ligands
3. Test the hypothesis that the cluster can be stabilized by protecting its surface with suitable bulky ligands that will effectively prevent it from reacting with adjacent clusters
4. In tandem with stabilization projects, students will attempt to enhance the cluster antimicrobial activity by conjugating it with penicillins and antiviral agents.
5. Investigate the feasibility of using the cluster as a template for protein synthesis by conjugating its carboxylic acid terminus with sequences of amino acids.
6. Conjugate the cluster suitable biological bases and investigate the possibility of using it as a template/sustrate for DNA replication.
7. Characterize the physical and chemical properties of the cluster.

The research will be performed at LACC's Chemistry facilities using existing analytical equipment including Nuclear Magnetic Resonance, Fourier Transform Infrared, and Ultraviolet-Visible absorption spectrometers. Promising samples will be further analyzed by outside collaborators for antimicrobial activity and characterization of material composition, mass, and structure.

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