# Crystal and Molecular Structures of New Metallocarboranes, $Au_{25}$ Gold Cluster and Metal Sensor Molecules

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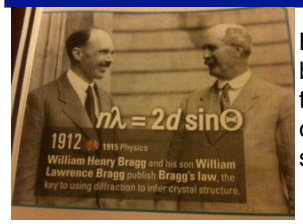
## Introduction




Bragg's equation has become one of the most trusted model used to calculate crystal structures.

Science **2014** *343*, 1092

2014 marks the 100th anniversary of Max von Laue's Nobel Prize for discovering that X-Rays fired into a crystal of copper sulfate produced a characteristic diffraction pattern.

2015 will be the 100th anniversary of the Nobel Prize to Bragg and Bragg for their equation that ultimately led to X-ray crystallography.

## Methods

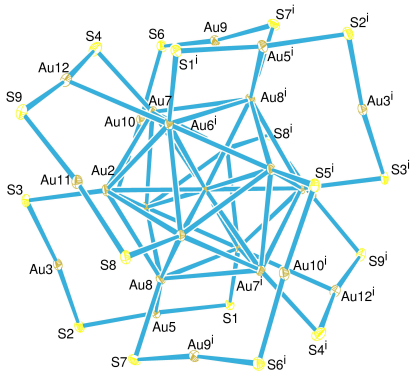
**SMART APEX II X-Ray Diffractometer**

## Results

Recently, we investigated complexed molecules which included: Metallocarboranes, $Au_{25}$ Gold Clusters and Metal Sensor Molecules.

Greater steps have been taken in-order to understand their molecular conformations thoroughly, and to generate optimal models as well as their applications.

Currently, our research group have been interested in the development of transition metal sensor molecules that can detect nerve gases, environmental pollutants and metal ions such as $Cu^{2+}$. We have also been actively involved in the formation of $Au_{25}$ Gold Cluster.

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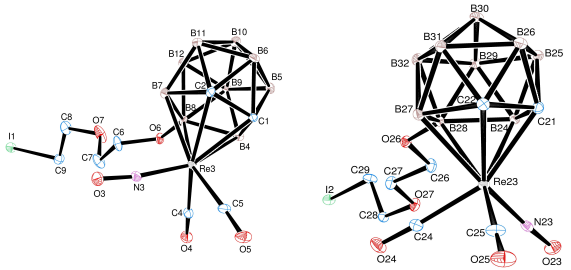
This is a very rare case of an icosahedral symmetric arrangement with 25 gold atoms at the center of the cluster.

Problem in this case is getting the complex as monodisperse sub-nanoparticles.

The crystal structure is crucial in showing that we produced the nanocluster, purified it, and verified its structure.

## Results

The synthesis of new metallocarboranes was formed by our collaborators at Saint Louis University, while the crystal and molecular structures was formed and studied at Western Michigan University, where we obtained the structures shown below.




Daniel Prùitt, Paul Jelliss, Dept of Chemistry, Saint Louis, MO

Transition metal Cu was detected in very small amounts, which makes it very sensitive and selective with other metals.

Attempts have been made to from a crystal of the Sensor-Metal complex attached to the molecule with no success to date.