Introduction to the Scientific Literature: Part 2

Reading and Understanding a Scientific Journal Publication

Refer to the research paper *J. Amer. Chem. Soc.* **2001**, *123*, 1625-1635 that was provided in Part 1.

The paper is written for experts within the field but incorporates basic, fundamental principles that you are familiar with, which in Part 2 relates to coordination chemistry. Your task is to find a number of informational points within the paper's details, relate them to your level of understanding, and answer questions designed around the chemistry of coordination complexes.

The importance of the paper relates to the destruction of chemical weapons of mass destruction, in particular, sulfur containing mustard gases.

The mustard gases were first used in World War I by the German army on different occasions in 1917 respectively against Russian, Canadian and French forces. The British were slower in their development of the mustards and first used the weapon in September 1918 against the Hindenburg Line. After World War I, enormous stockpiles of these and other chemical weapons were built up by many nations including the United States. The latest reported use of mustard agents was recently in Sudan. A global chemical weapons treaty barring their use and agreeing to their destruction was enacted in 1997.

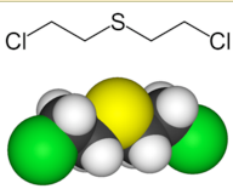
The destruction has become a major chemical challenge, not only because of the enormous numbers of weapons, but also because of the chemistry involved in the destruction. There are major environmental issues at stake, and important questions about the nature and toxicity of the chemical by-products produced from the destruction have drawn attention to the process and raised criticism of the plans to incinerate the chemical agents.

The U.S. Army, who sponsored the research in the publication, has undertaken the destruction of the U.S. chemical weapon arsenal. This paper deals with one aspect, which is to examine catalysts that employ oxygen from the air and ambient temperature to oxidize the major chemical in the stockpile, bis-(2-chloroethyl)sulfide, $ClCH_2CH_2SCH_2CH_2Cl$ ($C_4H_8SCl_2$).

For a detailed description of sulfur mustard gases see:
http://en.wikipedia.org/wiki/Sulfur_mustard

It is suggested that you refer to the questions on the reverse side of this page. Let the questions guide you as you go through the information.

Sulfur mustard (HD)



General	
Systematic name	Bis (2-chloroethyl) sulfide
Other names	Iprit Kampfstoff "Lost" Lost Mustard gas Senfgas Yellow Cross Liquid Yperite
Molecular formula	$C_4H_8Cl_2S$
Molar mass	159 g/mol
Appearance	Colorless if pure. Normally ranges from pale yellow to dark brown. Slight garlic type odor.
CAS numbers	[505-60-2] [39472-40-7] [68157-62-0]
Properties	
Density and phase	1.27 g/ml, liquid
Solubility in water	Negligible
Melting point	14.4 °C
Boiling point	217 °C
Vapor pressure	0.11 mmHg @ 25 °C

Name: _____

Introduction to the Scientific Literature
Part II: Coordination Chemistry

Refer to the handout and publication, *J. Amer. Chem. Soc.* **2001**, *123*, 1625-1635. Answer the following questions independently; this must be your work and yours alone.

Collaboration is not allowed for this part of the assignment.

1. a) Write a balanced equation for the reaction of $ClCH_2CH_2SCH_2CH_2Cl$ ($C_4H_8SCl_2$), plus $HAuCl_4$ plus $AgNO_3$?

   b) Name the compound: $HAuCl_4$ _____

2. How many compounds were made from the combinatorial library in the experiment that produced the catalyst?

3. What is the coordination number for the soluble gold catalyst?

4. What is gold's oxidation number in the catalyst?

5. What is the electron configuration of gold in the soluble complex, the likely molecular (VSEPR) shape of the gold complex, and the orbital hybridization?

6. What is the observed color of a Au(0) colloid of 65 nm particle size?

7. What is the approximate wavelength of the light being absorbed by the colloid in question #6?