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First Mercury and Silver Complexes of a Bulky Heterocyclic Thione Ligand

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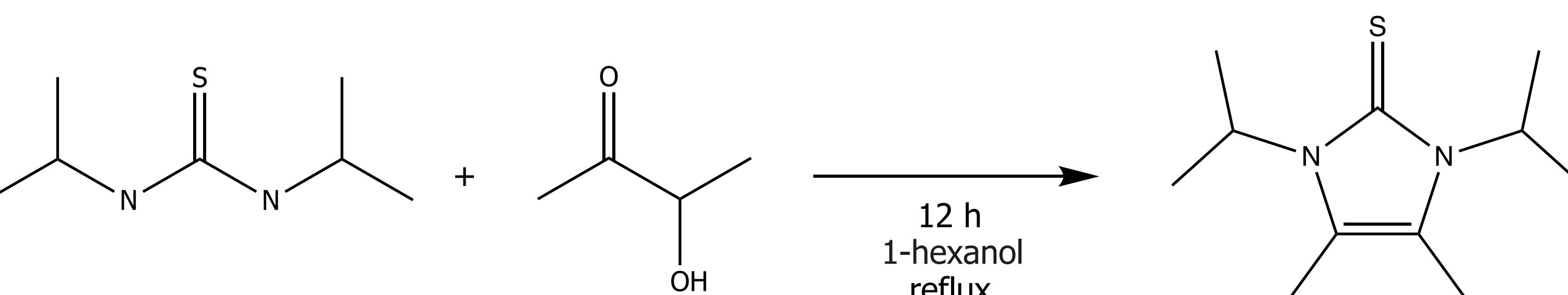


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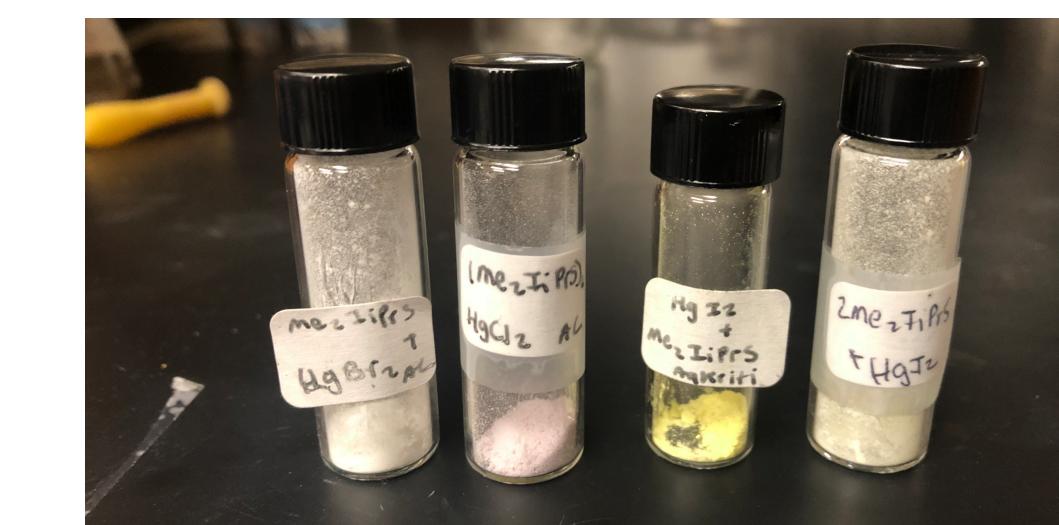
Abstract

The heterocyclic thione ligand Me_2LiPrS was first synthesized by Kuhn and Kratz in 1993, and has been subsequently used to prepare complexes for a variety of main group and transition metals, including aluminum, zinc, copper, rhodium, manganese, iron, cobalt, chromium, and nickel. We describe in this presentation our initial attempts to synthesize the first examples of mercury complexes with this ligand. More specifically, two separate series of mercury(II) complexes have been isolated, namely $(\text{Me}_2\text{LiPrS})_n\text{HgX}_2$ ($n = 1, 2$; $X = \text{Cl}, \text{Br}, \text{I}$). A discussion of the characterization data for these compounds, including nuclear magnetic resonance (NMR) spectroscopy data and elemental analysis is presented.

Synthesis of Me_2LiPrS Ligand

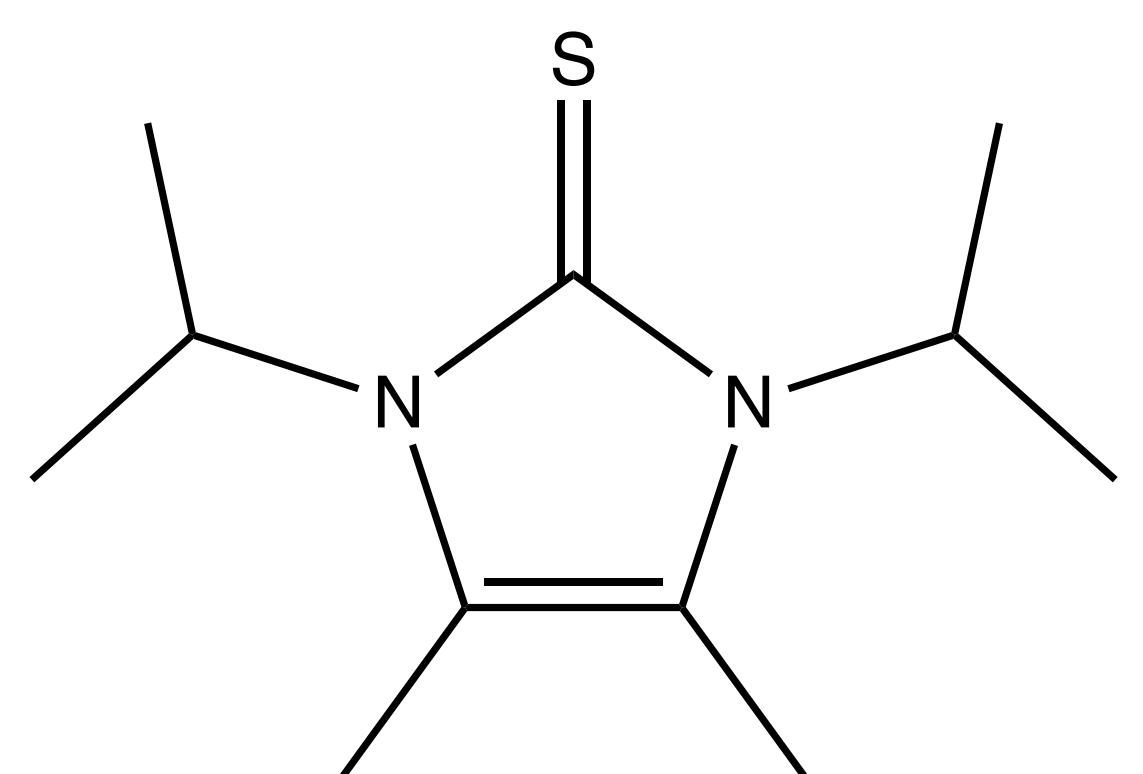


Mercury Complexes



- Mercury(II) compounds with two different stoichiometries (1:1 and 1:2) have been prepared; they are air-stable white or pale yellow solids
- The new complexes dissolve in polar organic solvents such as acetonitrile, DMSO, acetone, and methanol

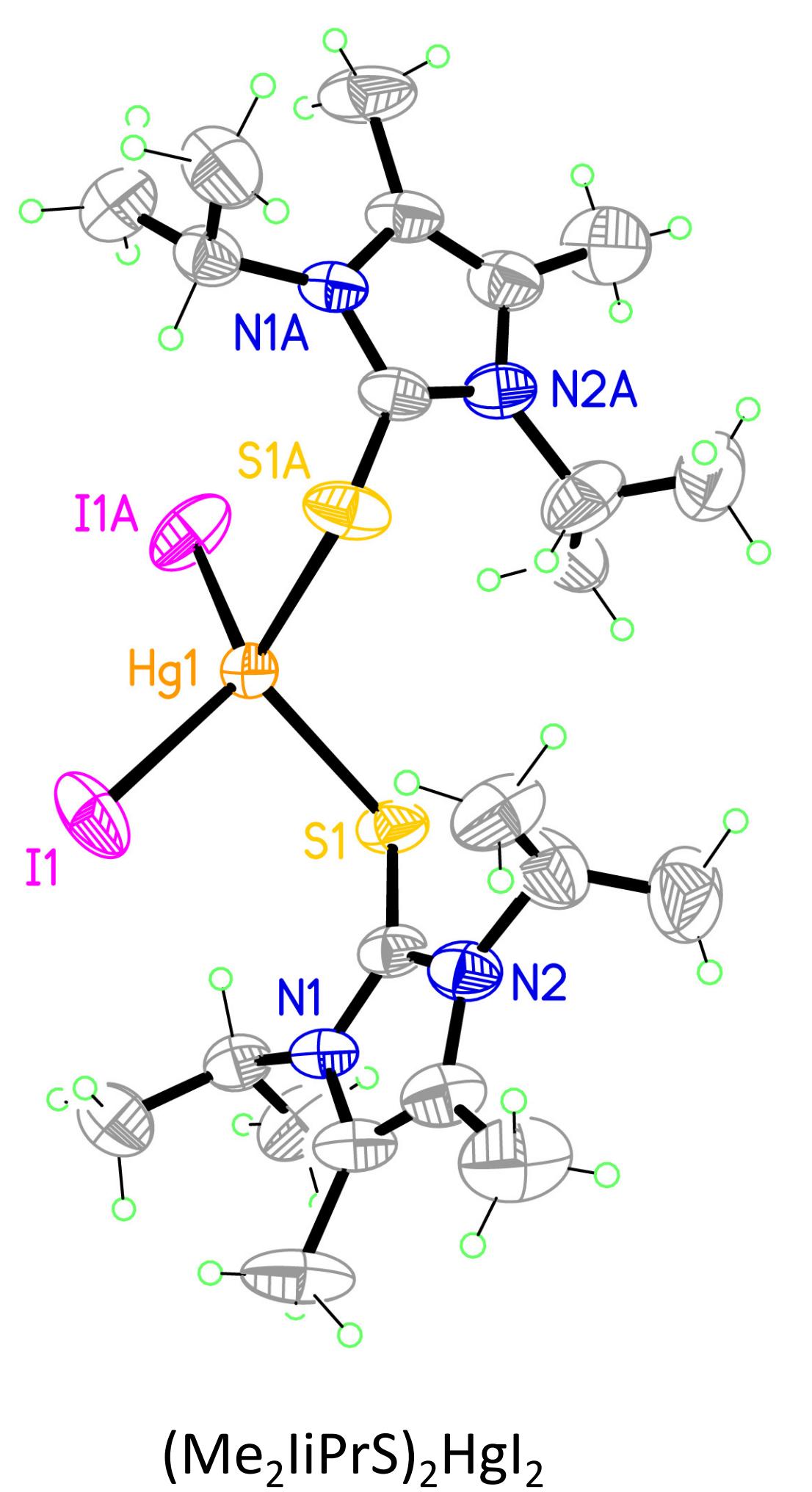
Heterocyclic Thione Ligand



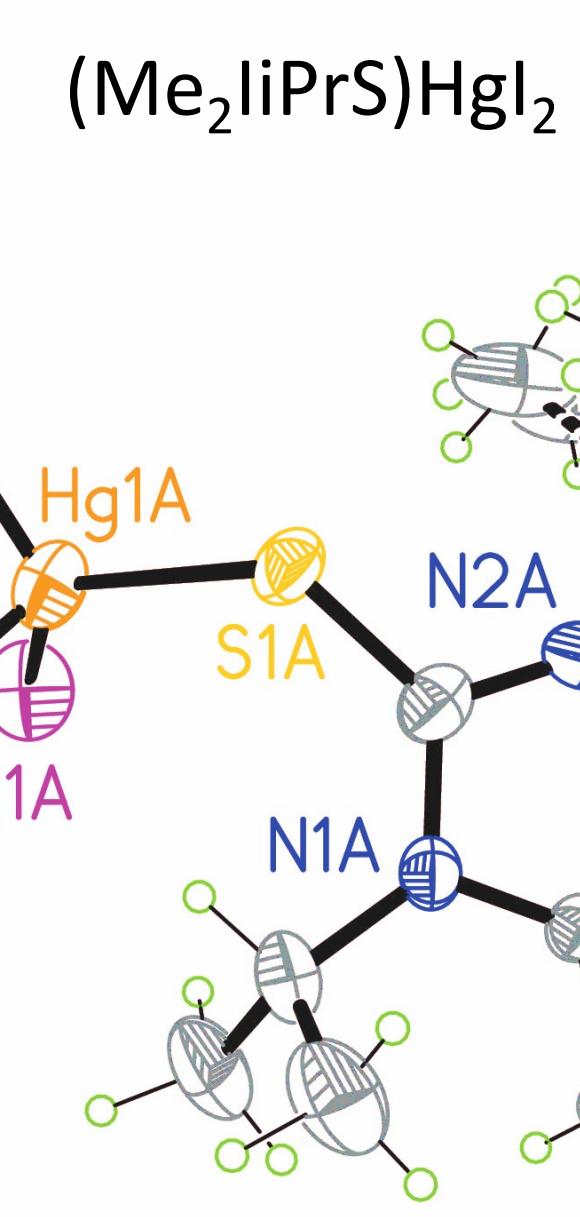
Me_2LiPrS

Me	methyl
I	imidazole
iPr	isopropyl
S	sulfur

Molecular Structures

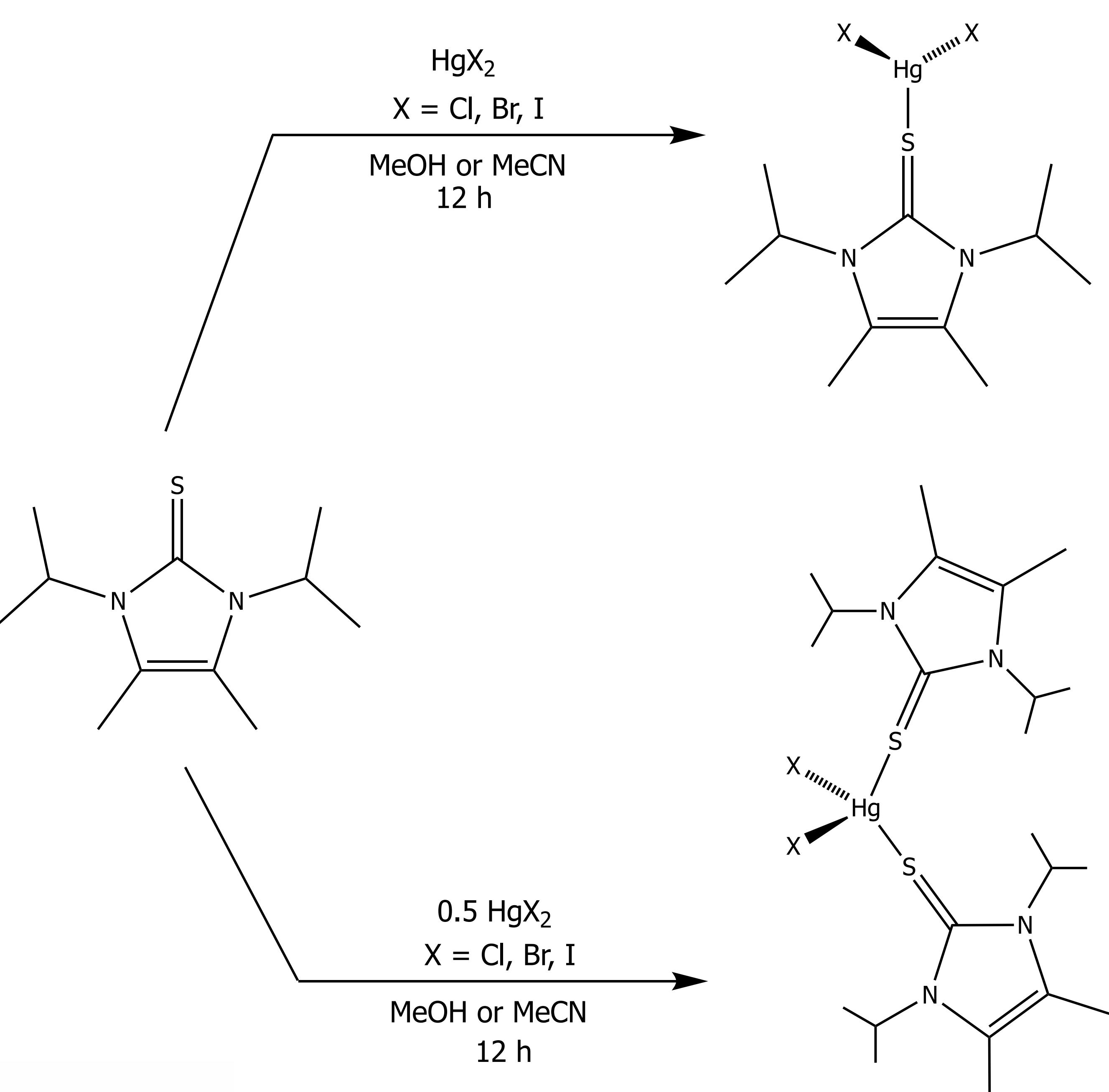


Selected bond lengths (Å) and angles (°)	
Hg-S	2.599 Å
C=S	1.758 Å
I-Hg-I	128.5°
S(1)-Hg-S(1A)	121.5°
S-Hg-I	100.6-109.2°



Selected bond lengths (Å) and angles (°)	
Hg-S	2.475 Å
Hg-I _t	2.680 Å
Hg-I _b	2.856 & 3.108 Å
C=S	1.714 Å
C-S-Hg	106.4°

Synthesis of Mercury Complexes



Current Progress

(Me ₂ LiPr)HgX ₂		
EA	Expt'l	X-ray
✓	✓	✓
		✓
(Me ₂ LiPr) ₂ HgX ₂		
EA	Expt'l	X-ray
X = Cl	✓	
X = Br		
X = I		✓

- Four out of 6 compounds have been characterized using elemental analysis
- Two compounds, specifically the two iodide compounds, have been crystallized
- Pending: infrared (IR) & ¹³C NMR data and melting points for the remaining compounds.

Conclusions

- The first mercury compounds with the Me_2LiPrS ligand have been prepared and their complete characterization is in progress
- X-ray crystallography has established that whereas the 1:2 complex $(\text{Me}_2\text{LiPrS})_2\text{HgI}_2$ is mononuclear, the 1:1 derivative $(\text{Me}_2\text{LiPrS})\text{HgI}_2$ is dinuclear and displays both terminal and bridging iodide ligands

Future Work

- Synthesize silver compounds with salts such as AgNO_3 , AgBF_4 and AgClO_4
- Study the biological activity (e.g., anticancer properties) of all the silver complexes

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