

# Synthesis, Characterization and the Oxidative Addition of Methyl Iodide to Cyclical Trinuclear Gold(I) Complexes

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## Introduction

Trinuclear gold(I) complexes are 9-membered rings formed by gold(I) centers with monoanionic ligands. In recent years these complexes have been studied for their luminescent and electronic properties; cyclical trinuclear complexes (CTCs) featuring pyrazolate and benzyl-imidazolate ligands have been observed to undergo oxidative addition resulting in a Au(I,III) mixed valence species. (Burini 2003).

Additionally, CTCs have been observed to undergo oxidative addition with the stepwise addition of dihalogens to gold centers. With this in mind, the goals of this research were to successfully synthesize and crystalize CTCs and perform the oxidative addition of methyl iodide to these complexes.

## Methods

### Synthesis of CTCs

The synthesis of all CTCs was completed under nitrogen atmosphere using standard Schlenk techniques. Various imidazoles were deprotonated with *N*-butyllithium in tetrahydrofuran. The lithiated imidazoles were then treated with dimethylsulphidechloro-gold(I) to produce the CTC.

### NMR and X-ray Crystallography

Nuclear Magnetic Resonance (NMR) spectroscopy and X-ray crystallography were used to analyze samples.

## Results

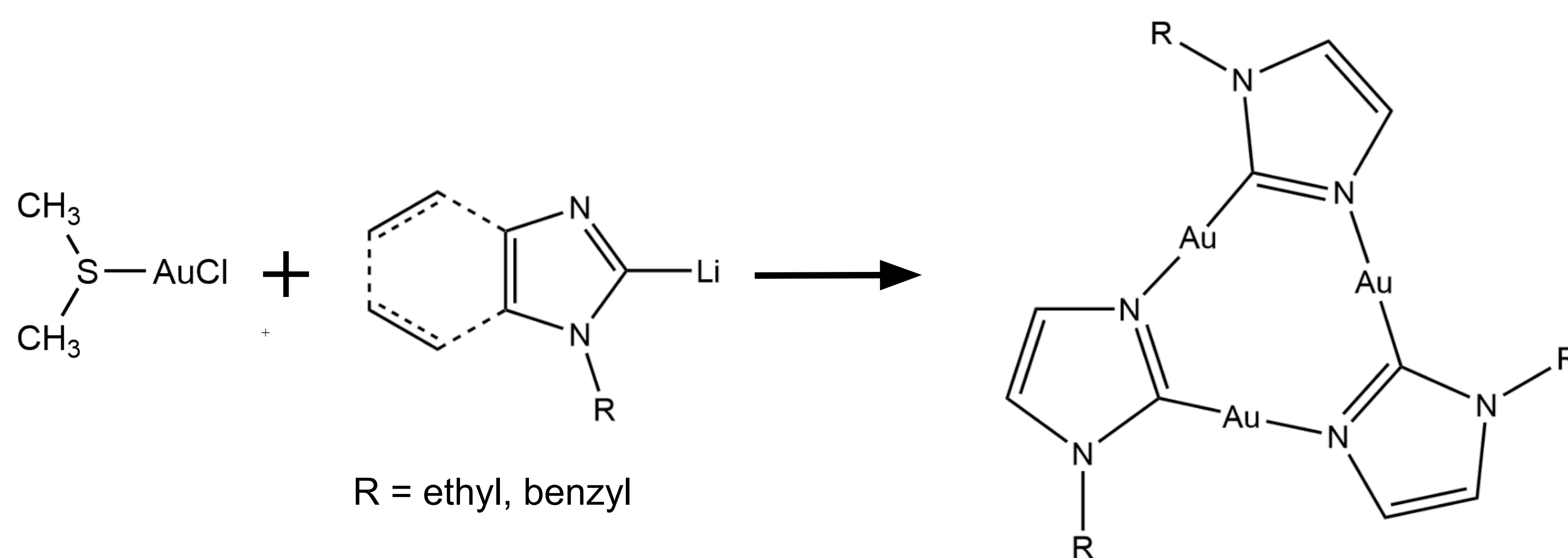


Figure 1: CTC Formation Reaction Scheme

Crystal Data	
Formula	C <sub>30</sub> H <sub>27</sub> Au <sub>3</sub> N <sub>6</sub>
Formula Weight	1062.47
Crystal System	Monoclinic
Space Group	P 2 <sub>1</sub> /n
a, Å	16.572(12)
b, Å	5.708(4)
c, Å	30.51(2)
α, deg.	90
β, deg.	99.419
γ, deg.	90
V, Å <sup>3</sup>	2847.(3)

Crystal Network	Bond Length (Å)
Au1-C11	2.02(3)
Au1-N21	2.05(2)
Au2-C21	2.00(3)
Au2-N31	2.05(3)
Au3-C31	1.95(3)
Au3-N11	1.98(2)
Au2-Au1	3.454(3)

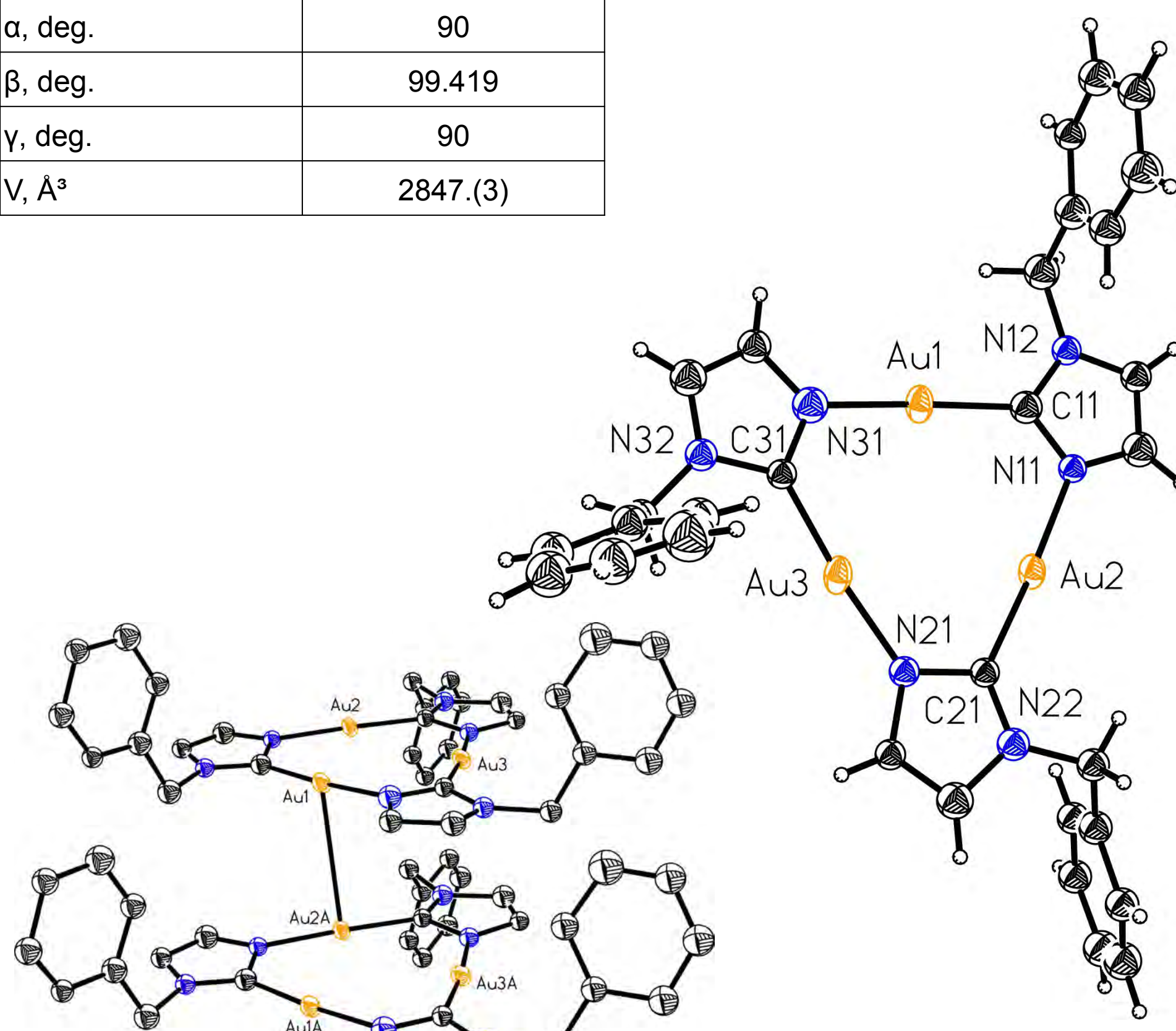


Figure 2: CTC (Benzyl) Crystal Structure and Crystal Data

Crystal Data	
Formula	C <sub>15</sub> H <sub>21</sub> Au <sub>3</sub> N <sub>6</sub>
Formula Weight	876.28
Crystal System	Monoclinic
Space Group	P 2 <sub>1</sub> /c
a, Å	17.9319(14)
b, Å	13.8237(11)
c, Å	15.7548(13)
α, deg.	90
β, deg.	103.25
γ, deg.	90
V, Å <sup>3</sup>	3801.4

Crystal Network	Bond Length (Å)
Au1-C11	2.002(8)
Au1-N31	2.085(7)
Au2-N11	2.059(7)
Au2-C21	1.995(8)
Au3-N21	2.035(7)
Au3-C31	2.012(8)
Au2-Au1	3.0702(4)

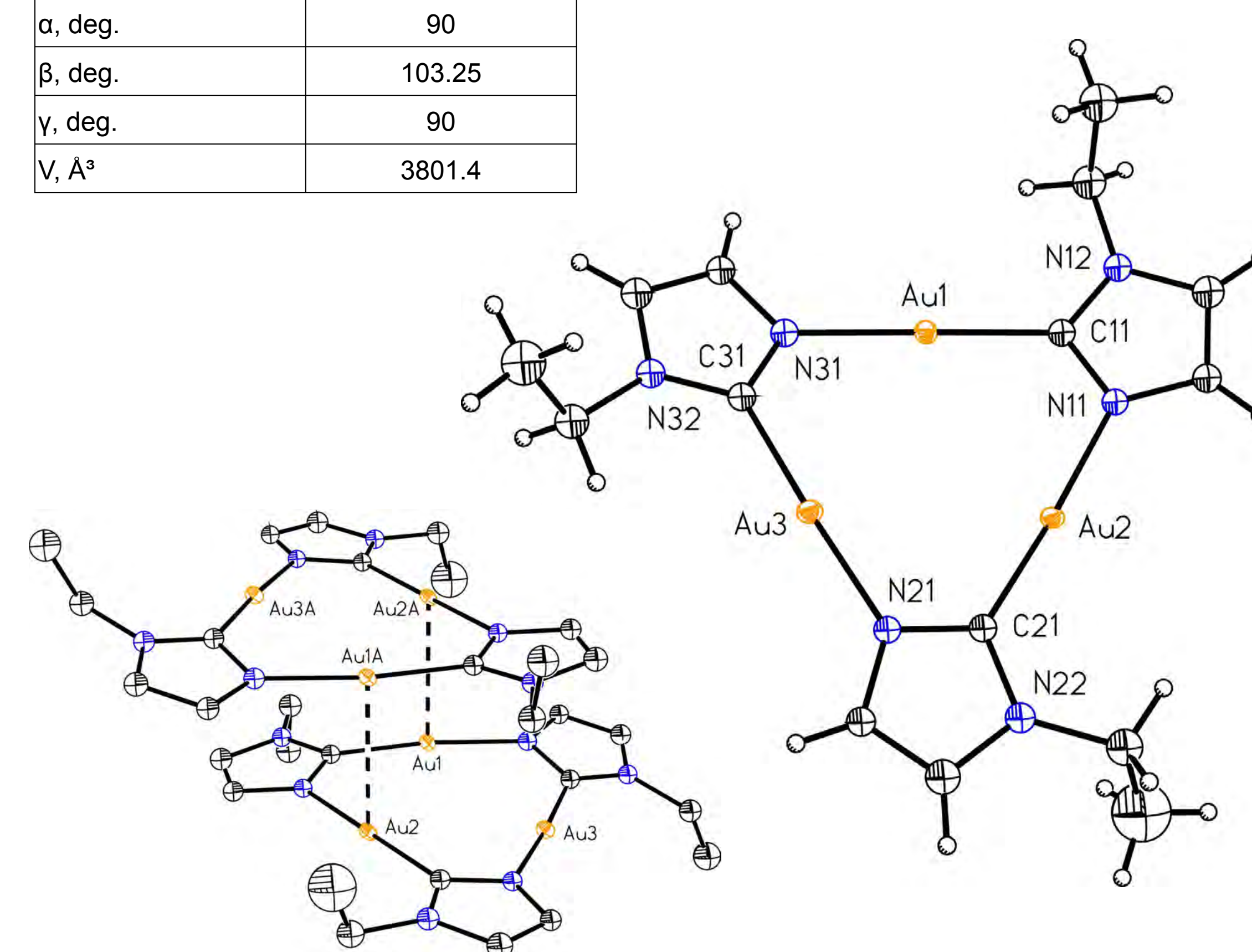


Figure 3: CTC (Ethyl) Crystal Structure and Crystal Data

## Conclusions and Next Steps

Going forward more CTCs using different imidazole ligands should be synthesized and their structures determined by X-ray crystallography, and different reaction conditions for the oxidative addition of methyl iodide to the CTCs will be investigated.

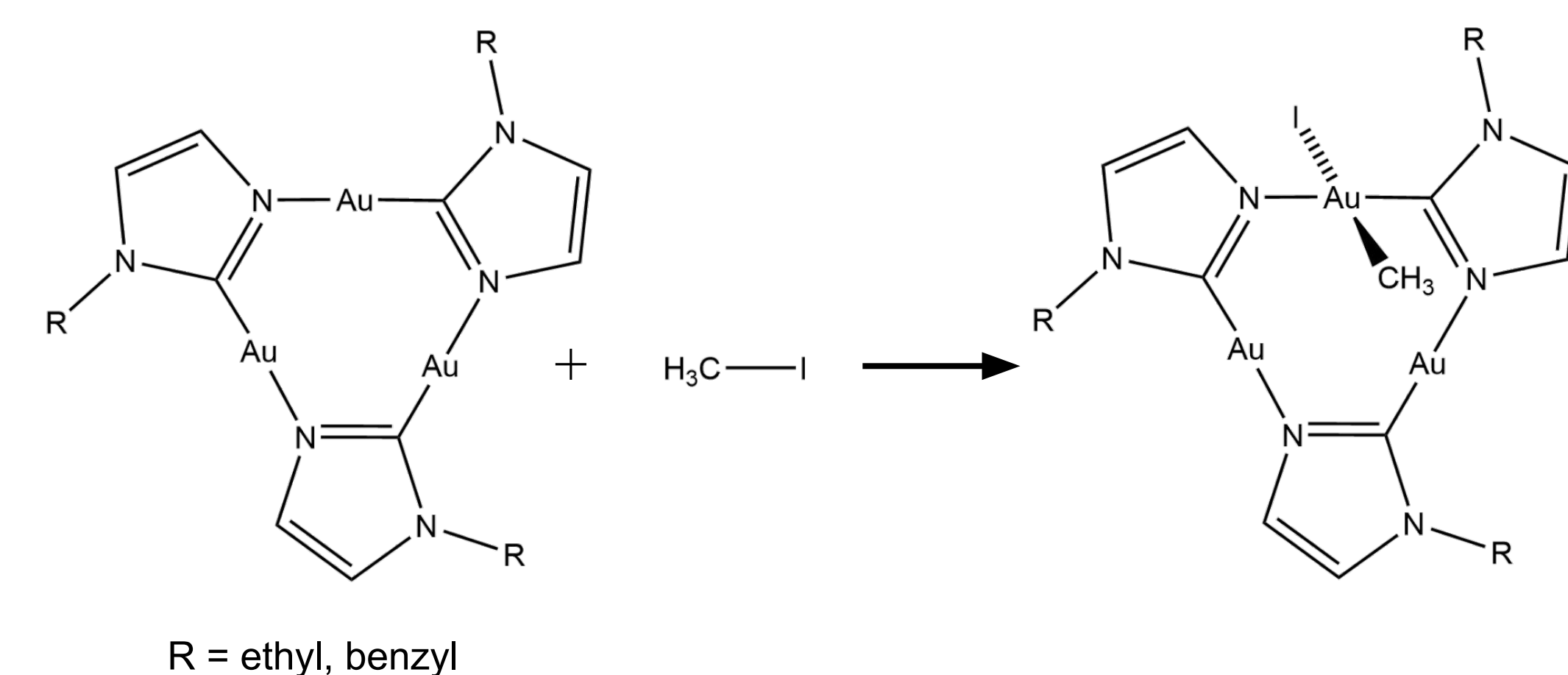


Figure 4: Proposed Oxidative Addition of CH<sub>3</sub>I to CTC Reaction Scheme (Next Steps)

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## References

1. Alfredo Burini, Ahmed A. Mohamed & John P. Fackler (2003): Cyclic Trinuclear Gold(I) Compounds: Synthesis, Structures And Supramolecular Acid-base Π-stacks, Comments On Inorganic Chemistry: A Journal Of Critical Discussion Of The Current Literature, 24:5-6, 253-280.
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