09.4-12 THE CRYSTAL STRUCTURE OF TETRA-N-BUTYLAMMONIUM TETRABROMOAURATE III. Jeffrey P. Johnson*, Physics Dept., Northern Ill. U., DeKalb, IL, 60115, USA. R. Brigitte Krause, Northern Ill. U., DeKalb, IL 60115, USA, and Elisabeth G. Sherry, Chemistry Division, Argonne Nat. Lab., Argonna, IL, 60439, USA.

Tetra-n-butylammonium tetrabromoaurate III, 

\[ \text{Br}_4\text{Au}^+ \text{N} \text{Bu}_4\text{N} \text{Br}^- \] crystallizes tetragonally with \( a=12.135(5) \) \( \text{Å} \) and \( c=8.508(4) \) \( \text{Å} \). Two formula units are contained in a unit cell of volume 1255\( \text{Å}^3 \). The probable space group is \( \text{P4/n} \). The structure was refined in space group \( \text{P4/n} \). It consists of discrete planar \([\text{AuBr}_4]^+\) ions which lie on fourfold axes and \([\text{Bu}_4\text{N}]^+\) ions which have \( 4 \) symmetry. The \([\text{Bu}_4\text{N}]^+\) ions are disordered with two distinct orientations for the carbon chains which are approximately mirror images of one another. The \( \text{Au-Br} \) bond distance is \( 2.40(1) \) \( \text{Å} \), the \( \text{N-C} \) distance is \( 1.56(2) \) \( \text{Å} \), and the \( \text{C-C} \) distances vary between 1.42\( \text{Å} \) and 1.58\( \text{Å} \). The final \( \text{R} \)-value for 1430 reflections was 0.092.

*now Physics Dept., Florida State U., Tallahassee, FL 32301, USA.

09.4-13 THE STRUCTURE OF A FOUR COORDINATE GOLD(I) COMPLEX: \( [\text{Au(PPh}_3)_2\text{SCN}]^- \). By J. A. Muir, M. M. Muir and S. Arias, Departments of Physics and Chemistry, University of Puerto Rico, Rio Piedras, PR 00931 USA, and C. F. Campana and S. K. Dwight, Nicely XRD Corp., 10061 Bob Road, Cupertino, CA 95014 USA.

Cryostals of several colorless gold complexes have been obtained by reacting \( \text{Au(PPh}_3)_2\text{SCN} \) with an excess of \( \text{PPh}_3 \) in benzene solution. \( [\text{Au(PPh}_3)_2\text{SCN}]^- \) is the first of these complexes whose crystal structure has been determined. It crystallizes in the space group \( P2_1/n \), with \( a = 15.806(6), b = 22.110(9), c = 15.774(4) \) \( \text{Å} \). The structure was solved using heavy atom methods, and refined with SHELXTL. For 4599 observed structure amplitudes, using data up to 2\( \theta = 45^\circ \), the final residuals were \( R = 0.066 \) and \( wR = 0.062 \). (\( \text{Au(PPh}_3)_2\text{SCN} \))

The coordination geometry about the gold is four-fold.

09.4-14 THE CRYSTAL STRUCTURES OF TETRAPYRIDINE COPPER(I) PERCHLORATE AND TETRAPYRIDINE SILVER(I) PERCHLORATE AT 250 K.

By K. Nilsson and Å. Öskarsson, Inorg. Chem. 1, Chemical Center, Box 740, S-220 07 Lund 7, Sweden.

This study has been carried out as part of a research programme on structural and thermodynamic features of complexes formed in pyridine.

In a preliminary communication Lewin, Michl, Ganis, Lepore and Avilizide (Chem. Comm., 1971, 1400) reported the crystal structure of \( \text{Cu(C}_{25}H_{34}O)\text{ClO}_4 \). We have redefined that structure and extended the measurements to the silver solvates. The compounds are isostructural, space group \( \text{P4} \) with \( Z=2 \) and \( a=12.471(3), c=6.894(4) \) and \( a=12.874(1), c=6.748(4) \) \( \text{Å} \) for the Cu and Ag compound, respectively.

Intensity data were collected at 250 K on a CAD-4 diffractometer using Mo-radiation. The reflexions converged to \( R=0.042 \) (Cu) and \( R=0.026 \) (Ag).

The structure is composed of discrete \( \text{H(C}_{25}H_{34}O) \) and \( \text{ClO}_4^- \) ions. The coordination geometry is tetrahedral with metal-nitrogen distances 2.047(4) \( \text{Å} \) and 2.322(3) \( \text{Å} \) in \( \text{Ag} \), while the Ag atom only 0.58 \( \text{Å} \) out of the least-squares plane through the P atoms.

The bond distances in these and other copper(I) and silver(I) compounds will be compared. For a given coordination figure, the difference between the distances \( \text{Ag-X} \) and \( \text{Cu-X} \) decreases markedly as \( X \) becomes softer.