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Preliminary communication

Dichloro(phenyl)di-n-propylgold(III) sulphide

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SUMMARY

An X-ray structure determination of the complex, $Au^{III}Cl_2(C_6H_5)$-n-Pr_2S, confirms the strong *trans*-influence of the σ-bonded phenyl group in square-planar gold(III) complexes.

Until the recent preparation by Liddle and Parkin[1] of a series of monophenylgold(III) complexes the only stable arylgold(III) compounds which had been characterized were with pentafluorophenyl ligands[2,3]. We have determined the structure of one of the reported monophenylgold(III) complexes, dichloro(phenyl)di-n-propylgold(III) sulphide.

The strong *trans*-influence of the σ-phenyl group, well characterized for square-planar complexes of a number of metals[4], has been confirmed in a gold(III) compound. The Au–Cl bond *trans* to the σ-phenyl group is 0.11 Å (7σ) longer than the *cis* Au–Cl bond.

Crystals of $AuCl_2(C_6H_5)S(n\text{-}C_3H_7)_2$ are monoclinic, with space group $P2_1/c$ with $a = 9.32(2)$, $b = 16.10(3)$, $c = 10.09(2)$Å, β 91.6°, V_c 1513Å^3; D_o 1.98, D_c 2.03g·cm^{-3}, $Z = 4$. The intensities of 1207 reflections (Mo-K_α) were estimated visually and the structure has been refined by block diagonal least squares to an *R*-value of 0.086 (Au, S and 2Cl anisotropic). The molecular structure and principal bond lengths (Å, e.s.d.'s in parentheses) are shown in Fig.1. The coordination is square planar with *cis* chlorine atoms. The phenyl ring is tilted at an angle of 64° to this plane.

The covalent radius of Au^{III} may be estimated as 1.28Å from the length (2.27Å) of the Au–Cl bond *cis* to the phenyl group (Cl radius 0.99Å). This gives an estimated length of 2.02Å for a Au^{III}–(σ-C_6H_5) single bond (C sp^2 radius 0.74Å) only 0.02Å longer than that observed. However the observed Au–C bond length (2.00Å) is 0.15Å shorter than the mean value of the Au–C_6F_5 bond lengths (2.18, 2.12(9)Å), found in $Au^{III}Cl(C_6F_5)_2PPh_3$,

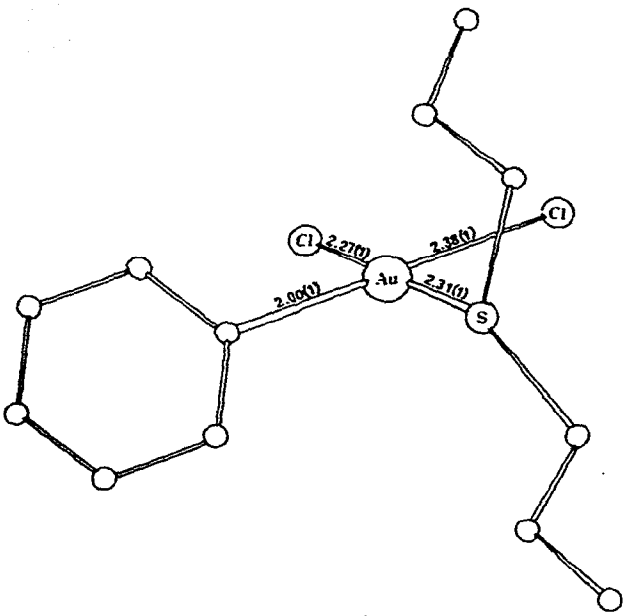

Fig.1. Molecular structure of $Au^{III}Cl_2(C_6H_5)$-n-Pr_2S

the only other arylgold(III) structure that has been reported[3]. This is consistent (although of only low significance) with the phenyl group being a better σ-donor than the pentafluorophenyl ligand. Similar effects have been observed in pentahalogenophenylnickel(II) compounds[5].

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