Intermolecular interactions in Au(I) and Au(III) complexes, Catharine Esterhuysen^{a*}, Stephanie Cronje^a, Helgard G. Raubenheimer^a and Gert J Kruger^b, ^aDepartment of Chemistry, University of Stellenbosch, Private Bag X1, Matieland 7602, Stellenbosch, South Africa, and ^bDepartment of Chemistry and Biochemistry, Rand Afrikaans University, PO Box 524, Auckland Park 2006, Johannesburg, South Africa. E-mail: ce@sun.ac.za

Keywords: Intermolecular interactions; Aurophilic interactions; Au(I) and Au(III) complexes

Au(I) complexes are well-known for forming aurophilic interactions, which are inter- or intramolecular Au...Au interactions with Au...Au distances shorter than 3.6Å [1]. Interactions between Au(III) atoms in neighbouring molecules are however much weaker, if they exist at all, with Au...Au distances often considerably longer than the sum of the van der Waals radii. Au(III)...Au(III) interactions thus very rarely play as important a role in directing packing as that observed for their Au(I) counterparts. Nevertheless packing in crystals of Au(III) complexes can be directed by other weak intermolecular interactions such as Au...halide. Au...S and even Au...π interactions. In this work the crystal structures of a series of Au(I) and Au(III) compounds illustrating these interactions are presented. A Cambridge Structural Database [2] analysis of similar structures is also included, which shows that although often much rarer than the aurophilic Au...Au interactions these interactions nevertheless play a role in packing that could lead to their use in crystal engineering methodologies.

^[1] S. S. Pathaneni, G. R. Desiraju J. Chem. Soc., Dalton Trans., 319-322, 1993.

^[2] F. H. Allen, Acta Crystallogr., B58, 380-388, 2002.