

ABSTRACT

In recent years, there has been a notable increase in interest in *N*-heterocyclic carbenes (NHC), which have emerged as a subject of considerable significance due to their strong σ -donating ability and steric features. These characteristics make them attractive ligands in transition metal complexes, with some NHC-metal complexes proving superior to their metal-phosphine counterparts. Among the transition metals where NHCs have been applied, NHCs-silver complexes have gained significant attention due to their simple synthesis, stability, fascinating structural diversity, and wide range of applications. Herein, a novel chelate mononuclear NHC-silver(I) was accomplished bearing a bisamide moiety in its backbone. Such mononuclear complex is synthesised using an equimolar ratio of the silver source and ligand precursor. Conversely, if an excess of the silver source was used, the reaction led to the formation of an unprecedented tetranuclear silver complex. Additionally, NHC-silver complexes have been recognised as effective carbene group transfer agents, enabling the synthesis of NHC complexes with other metals, such as nickel and palladium. These complexes exhibited chirality due to the coordination of the ligand to the metal centre in a helical manner. Both complexes were analysed in solid and liquid states, and DFT calculations were performed to understand the transition state and energy barrier of the configurational flip. The scope was extended with the synthesis of nickel and palladium complexes containing a larger side chain on the imidazole moiety, which proved to be more configurationally stable than their previous analogues. Furthermore, the synthesised NHC-silver complexes were also tested as antimicrobial agents, in which they demonstrated extraordinary properties. The minimum inhibitory concentration (MIC) values were as low as 1 $\mu\text{g/ml}$ and were active against Gram-positive bacteria, Gram-negative bacteria and Fungi. The silver complexes were also tested as catalysts in A^3 (aldehyde, amine, alkyne) and KA^2 (ketone, amine, alkyne) coupling reactions. The catalysts proved to be very reactive towards both coupling reactions with great overall yields and a wide tolerance for the substrate scope. Since A^3 coupling is a multicomponent reaction and with the good results presented by the complex, a small library of compounds was synthesised and was further used in data storage. Storage of data using small molecules remains a rather unexplored field. The use of the synthesised compounds proved to be suitable and efficient with a new cheaper and user-friendly approach being employed.