Concave halogen-bonding ligands for supramolecular structure

Multi-dentate ligands are of considerable importance in supramolecular architectures because of their strong affinity to the central atom and well-defined structures, as well as their control ability to the electronic structure. Crown-ether and cryptand are the typical examples where multi-dentate ligand plays a significant role in supramolecular chemistry. Many concave and macrocyclic ligands such as bipyridine and phthalocyanine are also known as constituents for functional organometallic compounds. On the other hand, multi-dentate ligand for halogen bonding is, to our knowledge, not known up to date, although halogen bonding is starting to attract recent attention [ref. 1]. Therefore we have synthesized multi-dentate halogen-bonding ligand in order to expand the chemistry of supramolecular assembly based on halogen bonding.

We have reported conducting nanowire and its sheath, both integrated in a crystal structure as shown in Figure 1 [ref. 2]. In these materials, convex type halogen bonding ligands have been used as building blocks for the insulating supramolecular assembly. In order to expand the variation of supramolecular architecture based on halogen bonding, we have synthesized concave ligand 1. Molecule 1 formed complex with halide ions which crystallized as tetraphenylphosphonium salts. The detail of the complex structure will be discussed in the presentation.

Ref.