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Structural Diversity of the Supramolecular Assemblies of Iso-Chalcogenazole *N*-Oxides and Their Derivatives

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Amongst the many molecules that are capable of forming chalcogen bonds, iso-tellurazole *N*-oxides stand out because of their ability to reversibly form macrocyclic aggregates that are persistent in solution.
Such structures are built from molecules linked by Te···O chalcogen bonds antipodal to the Te-N bond. Depending on crystallization conditions, tetramers and hexamers have been isolated. Their ability to act as macrocyclic ligands has been demonstrated with κ-Te complexes of late transition metal ions. In recent investigations, we have found a procedure that allows building a dodecamer that folds onto itself forming a cavitand that encapsulates certain solvent molecules such as cyclohexane, tetrahydrofuran and dioxane. The cyclic ethers promote binding of sodium cations which further stabilize the cavitand structure by binding oxygen atoms. Very different structures were obtained from Mg(II) salts. In this case, the metal is κ-O hexacoordinated. The iso-tellurazole oxide molecules remain aggregated, but the Te···O chalcogen bonds are trans to the Te-C bonds. This aggregate is, therefore, a new isomer if the hexamers known until now. These unprecedented structures denote the versatility of chalcogen bonding and invite further investigation to achieve full control of the supramolecular association of molecules of this family.
Introduction of an aromatic bridge between N and O gave a family of iso-tellurazolium *N*-phenoxides, which also assemble functional macrocyclic aggregates. More recently, we have explored replacing the O^- centre with Ar-N^- moieties to form iso-tellurazolium *N*-arylamides.