
In spite of large number contributions and advances in self-assembly of organic molecules based on noncovalent interaction, the area of organometallic compounds remains in this context largely unexplored. To date there has been no systematic attempt to exploit relationship between donor-acceptor interactions and hydrogen bonds though this relationship is of significance from material science to biochemistry. Both types of interaction are responsible for various types of self-organization and molecular recognition and without intimate understanding of cooperation between hydrogen bonds and classical donor-acceptor bonds will be difficult deduced general building principles for synthesis of self-assembly structures with well-defined properties.

In this report we present the structure investigation of the group 13 (M = Al, Ga, In) diorganometallic chelate complexes derived from simple α- and β-primary-amine alcohols. It will be demonstrated that group 13 amine-functionalized alkoxides may serve as an interesting model system for systematic study of interdependence between hydrogen bonds and classical donor-acceptor bonds will be difficult deduced general building principles for synthesis of self-assembly structures with well-defined properties.


Few proteins have undergone such detailed conformational analysis as bovine pancreatic trypsin inhibitor (BPTI), a 58 amino acid globular protein with three disulfide bonds, a well defined secondary structure and hydrophobic core. Several polymorphic forms have been reported for this protein and its mutants.

Recently, a room temperature, 1.42 Å resolution structure of a new tetragonal form (P4₁2₁2₁) has been reported from our laboratory for a strategic mutant with altered binding loop sequence. Many important features were observed in that structure such as: no change in the conformation of the binding loop despite three mutations, salt bridged N- and C-termini, a disulfide bond in two chiralities, five internal water molecules and four sulfate anions, an intermolecular four-stranded β-sheet, highlighting their role in the formation of very stable, highly diffracting crystal that can be grown on the time scale of hours.

Recently, low temperature (100 K), sub-atomic resolution (0.87 Å) data have been obtained for the same mutant crystallized under similar conditions. The structure has been refined with anisotropic displacement parameters using both conjugate gradient and least-squares algorithms in a way similar to small-molecule refinement. The final R factor is 10.74 % for all 46,219 reflections and 6,615 parameters. The overall structure is similar to that observed at room temperature with localized differences. Some of the high B-value residues have been resolved into double conformations, there are changes in the solvent region including appearance of cryoprotectant molecules and of additional ions. This low-temperature and high-resolution data allow a detailed analysis of intra- and intermolecular interactions involving not only the classical ones but also weak interactions, like N/C=H⋅⋅⋅p, and C–H–O hydrogen bonds.

In this presentation, a comparison of the room-temperature and low-temperature structures will be given and aspects of various intermolecular interactions and of their effect on local geometry will be discussed.