Some Hydrated Molecular Complexes of 4-Cyanophenylboronic acid: Significance of Water in the Structure Stabilization by Theoretical Investigations

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Introduction: Crystal engineering is a study of intermolecular interactions exhibited by molecules in their crystal structure and utilized its understanding in design of new compounds with desired properties. To understand and evaluate such interactions, computational power and quantum mechanical approaches have been explored such as Monte Carlo method, quantum-chemical coupled cluster techniques etc. For modeling this type of system one difficulty is to correctly include vdW interactions. Here we use DFT-D3 method.

Objective: To study intermolecular interactions present in molecular complexes of boronic acids experimentally and computationally using DFT-D3 method.

Methods: Molecular complexes of 4-cyanophenylboronic acid (4CyBA) with various aza donor coformers have been crystallized using slow solvent evaporation method.

Experimental: Crystal structure of complexes have been determined using single crystal X-ray diffraction technique.

Theoretical: Intermolecular interaction energies of synthons present in crystal structures have been computed using DFT, combined with D3-method by Grimme, implemented in NWchem-6.6. Simulations was carried out with B3LYP functional and 6-31++G(2d, 2p) basis set.

Outcomes:
- Single crystal analysis shows that though pure CyBA has anhydrate structure, it forms hydrates with various aza donor coformers.
- Binding energy simulations shows that water molecule form strong hydrogen bonds with CyBA as well as aza donors and play crucial role in structure stability.
- This study also highlights the CyBA as potential cocrystal former which has not been explored in crystal engineering field.

Future Work:
- By implementing the knowledge of intermolecular interactions formed by 4CyBA, currently we are working on plausible anhydrous forms of studied complexes using USPEX, Calypso.

Acknowledgement & References:
We are thankful to the computational resources provided by the Swedish National Infrastructure for Computing (SNIC) at HPC2N and PDC, and we acknowledge IIT Bhubaneswar for the financial support.