

International Conference on

Applied Crystallography

October 17-19, 2016 Houston, USA

Structure determination from powder diffraction data of self-assembled structures consisting of beta-peptide foldamers

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A well-designed beta-peptide foldamer can self-assemble to create various well-defined 3D architectures in aqueous solutions, named as foldecture. The term foldecture is combination of the words foldamer and architecture. Our group has reported unprecedented shapes of foldectures, such as a windmill and a molar tooth. These were highly homogenous both in terms of their size and in terms of morphology. Furthermore, to explore their potential use as functional materials, we recently published a study in which carboxyl groups were exposed to specific rhombic facets of foldectures. We found new potential capabilities of foldecture in relation to their mechanical properties as well as an anisotropic shape of a micro-sized container through the creation of a hollow cavity. Meanwhile, research on the functionalization of foldectures is expanding, as comprehending the self-assembly process and the resulting 3D shapes requires additional work. Hence, the structural determination of the molecular packing structure of foldecture is essential. In relation to this, the powder X-ray diffraction technique has been utilized here due to the dimensions and kinetically experimental conditions of foldecture. A PXRd analysis with synchrotron radiation was adequate to determine the packing structure with well-organized bonds and angle restraints. Further, it was able to designate the absolute orientation of the foldamers involved based on the predicted preferred orientation approximation. The use of a PXRd analysis on foldecture aided the understanding of the shape and properties of the newly formed foldecture and can be expected to play a major role in designing original examples of foldecture in the future.

Biography

Jintaek Gong has received his Bachelor of Science degree (Magna Cum Laude) in Chemistry from the Korea Advanced Institute of Science and Technology (KAIST) in 2011. He is now pursuing his Integrated MSc and PhD Program in the Department of Chemistry. He has published seven papers in reputed journals and has served as a Powder Crystallographer in the Biomimetic Organic Laboratory of KAIST.

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