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Abstract

Symmetry in Icosahedral Viruses: How It Is Exploited in the XFEL †

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We propose a new method of determining the structure of an icosahedral virus by exploiting the point-group icosahedral symmetry in the virus particle, which Caspar and Klug (1962) said was very common in virus structures [1]. The X-ray free-electron laser produces X-rays many orders of magnitude brighter than conventional X-rays, giving rise to speculation that it will enable structure determination of individual molecules or viruses without the need to form crystals. The problem is that the particles are presented to the X-ray beam in random orientations. Nevertheless, we show that exploiting the known point-group symmetry of the particles, it is possible to solve the structural problem by using an angular correlation method in an angular momentum representation. Note that we assume symmetry only in the construction of an oversampled diffraction volume from the correlations after the symmetry is revealed by objective means. The diffraction volume is dodecahedral (which has icosahedral point group symmetry). The reconstructed real-space image obtained from an oversampled diffraction volume by an iterative phasing algorithm, is icosahedral.

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Reference

1. Caspar, D.L.D.; Klug, A. Physical principles in the construction of regular viruses. *Cold Spring Harb. Symp. Quant. Biol.* **1962**, *27*, 1–24.