

11.4. DENZO AND SCALEPACK

created when data from a new detector appear or when the detector is rebuilt, which is done rarely, typically by the X-ray equipment administrator. The instance of the experiment allows for data from more than one crystal of the same space group. The uniform series of diffraction images form 3D groups. There is no limit to the number of 3D groups and, in the case of non-uniformity in the series (*e.g.* found during data analysis), the 3D group can be split into two or more smaller 3D groups. The smallest 3D group can consist of one image. The crystal instance contains a set of 3D groups with a relative orientation and exposure level known *a priori*. In practice, this means that data contained in a single crystal instance were collected from one sample at one site with potentially different settings of goniostat, data-collection axis, crystal translation, detector position, detector mode (*e.g.* binned/unbinned) or exposure level.

11.4.11. Final note

The methods presented here have been used to solve a great variety of problems, from inorganic molecules with 3 Å unit-cell

parameters to a virus of 700 Å diameter which crystallized in a $700 \times 1000 \times 1400$ Å cell. The most important test, stressing the precision and robustness of the method, is the successful application of the programs to many multiple-wavelength anomalous dispersion structure determinations.

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