MS38 Computations with/for Pair Distribution Functions

MS38-03
Symmetry-Adapted Pair Distribution Function Analysis
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Abstract
Symmetry-Adapted Pair Distribution Function Analysis (SAPA)[1] is a novel technique for obtaining information on local dynamics and disorder from pair distribution function (PDF) data of crystalline materials. In the SAPA method, the crystal structure is expanded to a supercell of a given size and then broken down into a symmetry-mode basis using the *ISODISTORT* online software. Using the TOPAS command line functionality, groups of modes transforming as the same irreducible representation can be tested in turn, in order to find the modes most responsible for any deviation of the local structure from the average. With the python programming language, this technique can be performed as an automated process. Using this method, we have been able to elucidate the underlying symmetry of the successive ferroelectric phase transitions in $BaTiO_3$[2] and have highlighted the importance of structural flexibility in determining the range and magnitude of negative thermal expansion in ReO_3[3] and related structures[4].

References
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A flowchart of the steps for the SAPA method