Crystallography online by the Bilbao Crystallographic Server

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Databases & Retrieval Tools

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INTRODUCTION

The Bilbao Crystallographic Server is a free web site with crystallographic databases and programs. The server gives access to the databases containing the data from the International Tables of Crystallography vol. A, Space Group Symmetry, vol. A1, Symmetry Relations between Space Groups and vol. E, Subperiodic Groups. The server provides very useful information in studies related with crystal-structure symmetry, phase transitions and solid state problems.

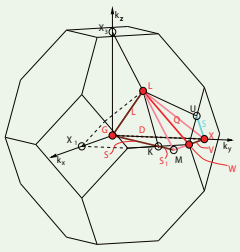
The available software is divided in several shells according to different topics:

- Simple Retrieval Tools
- Goup-Subgroup Relations
- Space Group Representations
- Solid State problems
- Structural Tools

Bilbao Crystallographic Server main page

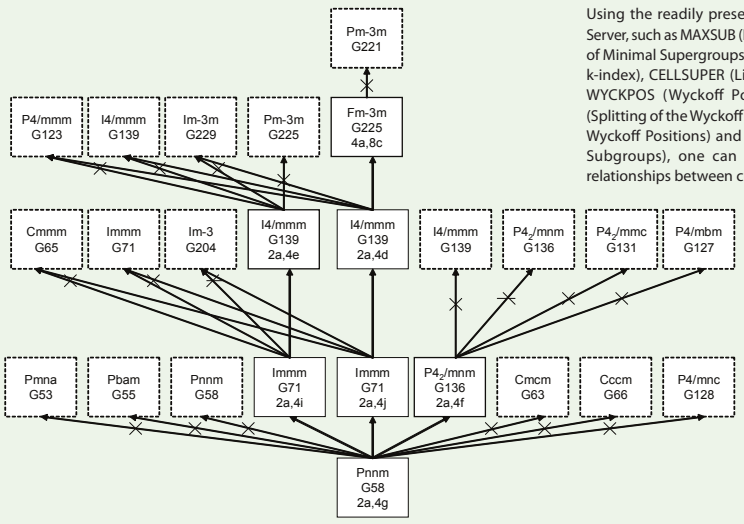
ACCESS TOOLS TO DATABASES

GENPOS	General Positions
WYCKPOS	Wyckoff Positions
WYCKSETS	Wyckoff Sets
NORMALIZER	Normalizers
KVEC	Wave vector types
HKLCOND	Reflection conditions
MAXSUB	Maximal Subgroups
SERIES	Isomorphic Subgroups
SYMMETRY OPERATIONS	Geometric Interpretations



KVEC contains a classification of wave vectors and Brillouin zones for the space groups. In the graph the Brillouin zone of the space group Fm3m (225) with all its special wave vectors.

APPLICATIONS: CRYSTAL STRUCTURE RELATIONSHIPS



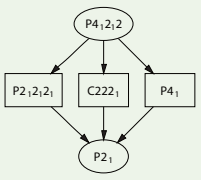
Using the readily present tools in the Bilbao Crystallographic Server, such as MAXSUB (List of Maximal Subgroups), MINSUP (List of Minimal Supergroups), CELLSUB (List of subgroups for a given k-index), CELLSUPER (List of supergroups for a given k-index), WYCKPOS (Wyckoff Positions of Spacegroups), WYCKSPLIT (Splitting of the Wyckoff Positions), WYCKSETS (Equivalent sets of Wyckoff Positions) and SUBGROUPGRAPH (Lattice of Maximal Subgroups), one can explore, construct and visualize the relationships between crystal structures.

The ascending group-subgroup tree for the Pnnm (G58) : 2a, 4g (e.g., MeO2 ; Me: Cr, Ge, Mn, Pt, Ru, Sn)

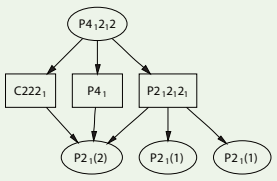
Group-Subgroup Relations

LATTICE OF MAXIMAL SUBGROUPS

SUBGROUPGRAPH provides the basic tool for the study of group - subgroup relations between two space groups G > H of index i. The result of the program includes chains of maximal subgroups between G and H, the determination of all different subgroups H_j of type H and index i and their distribution into conjugacy classes.



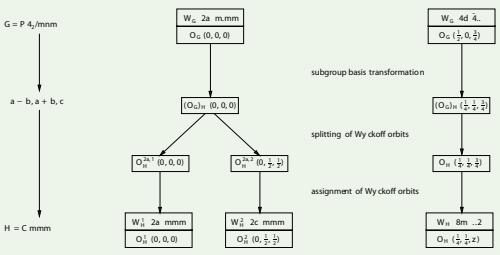
The contracted graph for $P4_12_12$ (92) > $P2_12_12_1$(4), index 4. The nodes correspond to space group types. The edges represent the possible group-maximal subgroup pairs.



The complete graph for the lattice of maximal subgroups of $P4_12_12$ (92) > $P2_12_12_1$(4), index 4. The three P21(4) subgroups are distributed in two classes of conjugate subgroups.

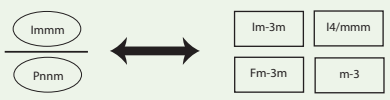
WYCKOFF POSITION SPLITTING

WYCKSPLIT obtains the relations between the atomic orbits of a group-subgroup pair G > H. In the graph: the splitting of the Wyckoff positions 2a and 4d of the group $P4_2/mnm$ into the subgroup Cmmm.



COMMON SUBGROUPS/SUPERGROUPS

COMMONSUBS / COMMONSUPER calculate the common sub/super groups of the given space groups for a designated maximum k-index.

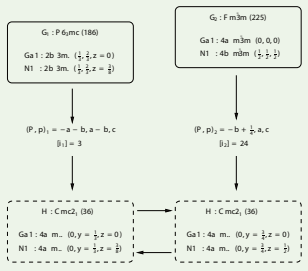


TRANSITION PATHS

TRANPATH calculates the possible transition paths between two structures with no group-subgroup relation between their phases. Given the two structures specified by their space groups, lattice parameters, and the atomic coordinates in the asymmetric units, the program calculates the set of transitions paths of maximal symmetry.

Symmetry conditions on maximal transitions paths:

- A common subgroup H of the two symmetry groups.
- The compatibility of the occupied Wyckoff orbits in H.
- H has maximal symmetry.



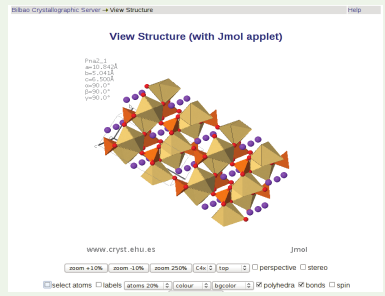
General Scheme: Wurtzite to Rocksalt transition path.

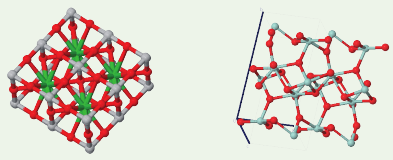
Visualization

VISUALIZE

With VISUALIZE, you can easily have a 3D visual representation of your structure, whether to demonstrate it in a seminar, course, anywhere, independent of your operating system as long as you have an access to the internet. Fully supporting CIF format.

Non-standard settings can also be visualized via transforming it first through SETSTRU and then switching to VISUALIZE.

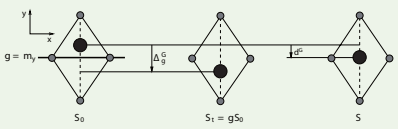




Solid State Applications

PSEUDOSYMMETRY SEARCH

PSEUDO performs systematic search for pseudosymmetry. For a specified crystal structure the program search for pseudosymmetry with respect to its supergroups G_i. The structure is considered pseudosymmetric if the atomic displacements relating the hypothetical phase to the experimental phase are smaller than a previously chosen tolerance factor.

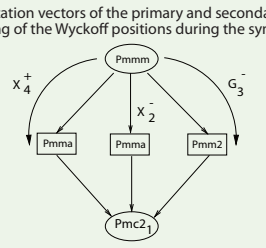


The pseudosymmetry search (PSEUDO) method scheme.

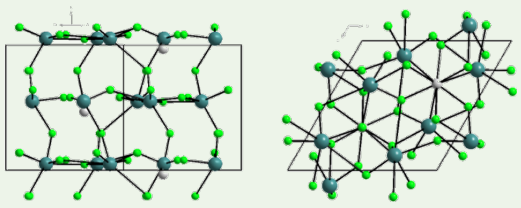
SYMMETRY MODES

SYMMODES realizes a group-theorethical analysis of a structural phase transition characterized by a symmetry change from G to H, with G > H. Given the symmetry groups G, H and the index i the program constructs the lattice of maximal subgroups. For a chosen subgroup and specified the occupied Wyckoff orbits, the program calculates :

- The polarization vectors of the primary and secondary modes
- The splitting of the Wyckoff positions during the symmetry break.



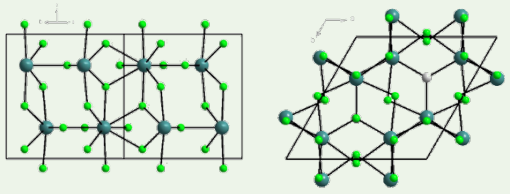
Symmetry modes for Pmmm(47) > $Pmc2_1$ (26), index 4



Above: *The experimental $P6_3$ structure of $NaSb_3F_{10}$.*

Below: *The $P6_3/mmc$ structure obtained with PSEUDO as ideal symmetrized configuration of the same compound.*

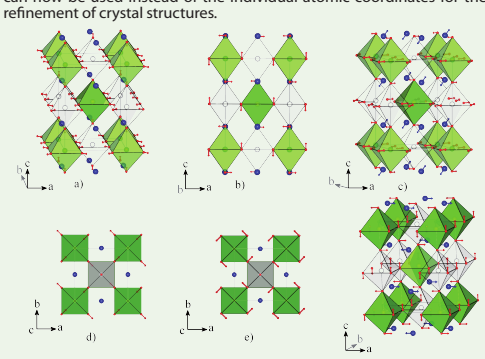
The maximal atomic displacement of the displacive distortion relating the two structures is of the order of 0.64Å.



AMPLIMODES

If the studied crystal is pseudosymmetric it can be seen as a result of a distortion with respect to a higher symmetry configuration. AMPLIMODES calculates all posible symmetry modes participating on the symmetry break and decomposes the distortion in terms of the modes. The nature of these symmetry modes makes them an ideal basis to describe the distortion. The hierarchy shown by these symmetry modes and the essencial invariance of their polarization vectors with the variation of external conditions can be very useful for the refinement of this type of structures, specially when the data are insufficient or of low quality.

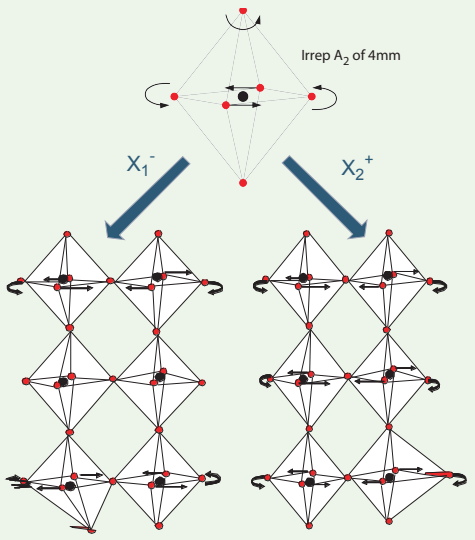
A new feature added to AMPLIMODES allows the generation of input files for FullProf which has been adapted so that symmetry-mode coordinates can now be used instead of the individual atomic coordinates for the refinement of crystal structures.



The symmetry-mode analysis performed on the C2/m and P2₁/c structures show that the relevant symmetry modes on this symmetry break are those associated to the irreps G_1^+,G_4^+ and X_3^+. So, if the refinements are done using these modes while fixing the rest, the complexity of the calculation will be reduced without adding too much error.

SITE SYMMETRY

SITESYM establishes symmetry relations between the localized states (local atomic displacements) and crystal extended states (phonons, electrons, etc.) over the entire Brillouin zone. Given the space group symmetry and the occupied Wyckoff positions the program determines the character of the induced representations of the site symmetry group.



Crystal extended modes induced by BO_6 octahedra rotations in Aurivillius compounds