10, 12 and 16 carbon atoms were solved using parallel tempering and refined against X-ray powder diffraction data using the Rietveld method. The azetidinone ring in the three compounds display a pattern of asymmetrical bond distances and an almost planar conformation, these characteristics are compare with periodic solid-state and gas phase DFT calculations. The compounds form 1-D, 2-D and 3-D networks of H-bonds of the type N—H•••O (and C—H•••O) as their side-chain augment. The compounds pack as corrugated sheets, separated by approximately 4.40 Å, which piled up along the [0 0 1] direction

R= (I)   Decyl
(II) Dodecyl
(III) Hexadecyl
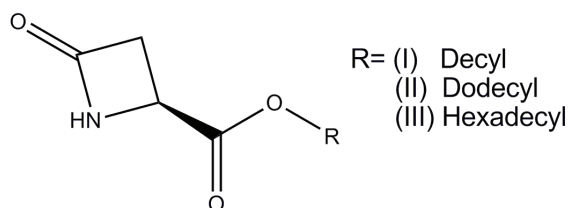
Keywords: powder diffraction; structure solution; β-lactams

Solving Crystal Structures Using Symmetry-Mode Collective Coordinates. <u>Danel Orobengoa</u>[a], Juan Rodriguez-Carvajal[b], Juan Manuel Perez-Mato[a], Mois I. Aroyo[a], Abdessamad Faik[c], Josu Mirena Igartua[c]. [a]*Dpto. Física de la Materia Condensada, UPV, Bilbao, Spain.*[b]*Diffraction Group, Institut Laue-Langevin, Grenoble Cedex 9, France,* [c]*Fisika Aplikatua II Saila, Zientzia Fakultatea, Euskal Herriko Unibertsitatea, Bilbao, Spain.*
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The computer program Amplimodes performs symmetry-mode analysis of any pseudosymmetric structure and it is freely accessible on the Bilbao Crystallographic Server (www.cryst.ehu.es) [1]. A new option, recently added to Amplimodes, allows automatic generation of input files for FullProf[2]. The refining program has also been adapted to work with the basis of symmetry modes constructed and used by AMPLIMODES. This allows performing crystal structure refinements using symmetry-adapted collective coordinates as refinable parameters. This represents a new way of treating the experimental diffraction data that captures the physics of these structures, which in many cases are the result of real or virtual phase transitions.
If the studied structure is pseudosymmetric, it can be seen as the result of a distortion with respect to a higher symmetry configuration. The space groups of the reference G and the distorted H structures are group-subgroup related (G>H). AMPLIMODES lists all the possible symmetry modes participating in the distortion. Their components are referred to the unitary basis of the H phase. Thus, the coordinates of the atoms on the H phase can be written as: $r_i(H)=r_i(G)+\Sigma_m (A_m \varepsilon(m,i))$, where $r_i(G)$ are the ideal atomic coordinates of the G phase referred to the H basis and A_m and $\varepsilon(m,i)$ are the amplitudes and the polarization vectors

of the symmetry modes. The set of polarization vectors $\varepsilon(m,i)$ is provided by the file produced by AMPLIMODES, and A_m are the collective coordinates refined by FullProf, substituting the individual atomic coordinates.
This approach can be very useful for determining low symmetry structures with strong pseudosymmetry [3]. A hiearchy is expected among distortions of different symmetry as well as an essential invariance of their polarization vectors with the variation of external conditions (temperature, pressure, etc.), making the refinement more robust and stable when the data are insufficient or of low quality (e.g. powders or twinned crystals).
In this communication the method will be presented in more detail and illustrated with a few examples.

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Keywords: refinement; symmetry-modes; bilbao crystallographic server

Crystal Structure and Superconducting Properties in YNi$_{2-x}$M$_x$B$_2$C (M = Al, Cr, Co). <u>Antoni Winiarski</u>[a], Anna Winiarska[a], Andrzej Ślebarski[a], Zofia Drzazga[a], August Chełkowski[a]. [a]*Institute of Physics, University of Silesia, Uniwersytecka 4, 40-007 Katowice, Poland.*
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Superconductivity, magnetism and structural properties of RE(Ni$_{1-x}$Me$_x$)$_2$B$_2$C (RE – rare earth metal, Me – metal) have been studied by several authors, e.g. [1], [2], [3]. Polycrystalline YNi$_{2-x}$M$_x$B$_2$C (M = Al, Cr, Co) samples were prepared by arc melting under Ar atmosphere and annealed at 1323 K for 100 hours. The stoichiometry and homogeneity of the samples were checked by XPS method. The samples with small values of x are superconductors. They crystallize in the tetragonal space group I4/mmm. Temperature dependence of the lattice parameters was measured in the temperature range from 12 K to 297 K using a Siemens D5000 X-ray Diffractometer with Cu$_{Kalpha}$ radiation. The Rietveld method was applied to calculate the crystal lattice parameters. Electrical resistance and transition temperature to superconductivity T$_c$ were measured using four-probe method in the temperature range of 4.2 K – 297 K. We found anomalies in change of the lattice parameters in YNi$_{2-x}$Co$_x$B$_2$C for the x parameter less than 0.03. The change in the lattice parameters is hardly visible in the x range 0 – 0.03. We suggest explaining observed effect in the term of crystal lattice defects. The lattice parameters for YNi$_{2-x}$Co$_x$B$_2$C samples with $x > 0.3$ decrease linearly in the superconducting region.

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Keywords: borides; powder diffraction analysis; superconductors