

HANDS-ON SESSION: CRYSTALLOGRAPHY ONLINE BY THE BILBAO CRYSTALLOGRAPHIC SERVER

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The Bilbao Crystallographic Server (www.cryst.ehu.es) is a website with crystallographic databases and programs. It can be used free of charge from any computer with a web browser via the Internet. The hands-on session aims to give a practical guide to some of the online computer tools available on the Bilbao Crystallographic Server for treating problems of theoretical crystallography, solid-state physics, and crystal chemistry. The following topics will be discussed in more detail: (i) coordinate transformations in crystallography with special emphasis on the computer tools for crystal-structure descriptions and crystal-structure comparisons; (ii) crystallography of structural phase transitions; (iii) symmetry relations between crystal structures and their descriptions by Baernighausen trees (family tree of structures); (iv) evaluation of structural pseudosymmetry with applications in the search of ferroic materials.

The hands-on session will include brief presentations of the computer tools followed by exercises illustrating their practical applications in case studies.