Oral Contributions

[MS44-03] Bilbao Crystallographic Server: New Tools and Improvements M. I. Aroyo[a], J. M. Perez-Mato[a], E. S. Tasci[b], G. de la Flor[a], S. Gallego[a], L. Elcoroa and G. Madariaga[a]

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The Bilbao Crystallographic Server (http://www.cryst.ehu.es) website offers crystallographic databases and programs [1,2]. It can be used free of charge from any computer with a web browser via Internet. The server has been operating for more than ten years, and new programs and applications are constantly being developed. The aim of the present contribution is to report on the current state of the server emphasizing on the newly developed computer tools and the underlying crystallographic algorithms. The utility of the available applications will be demonstrated by illustrative examples. The server is built on a core of databases that include data from International Tables, Vol. A: Space-group symmetry, Vol. A1: Symmetry Relations between Space Groups and Vol. E: Subperiodic groups. A k-vector database with Brillouin-zone figures and classification tables of the wave vectors for all 230 space groups is also available. Recently, a Magnetic Space Groups database with general positions and Wyckoff positions in both OG and BNS notations, alongside with a new tool for the calculation of systematic absences have also been incorporated into the server [3]. There are a number of online applications essential for problems involving group-subgroup relations between space groups and their irreducible representations. The database of incommensurate structures, hosted by the server, contains both single-modulated structures and composites. A set of recently developed structure-utility programs includes basic tools for transformations between different structure descriptions as for example, switching between different settings or structure transformations compatible with a specific symmetry reduction. The server offers an online tool for a quantitative analysis of the similarity of two structure models, also helpful for the recognition of identical or nearly identical atomic arrangements of different compounds. There is a program for the study of structure relations between two phases of the same compound with group-subgroup related space groups. The tool is of great utility for the construction of family trees of homeotypic crystal structures, known as Baernighausen trees. Parallel to the crystallographic software there are a number of programs facilitating the study of specific problems related to solid-state physics, structural chemistry and crystallography. There are online tools for evaluation of the pseudosymmetry of a given structure, for group-theoretical analysis of structural phase transitions or for the determination of phonon extinction rules in inelastic neutron scattering and diffuse scattering experiments. Of special interest is a set of newly developed tools for the analysis of the infrared and Raman activity of phonon modes at the Brillouin-zone centre, including the calculation of selection rules of infrared, Raman, hyper-Raman and second-order processes, or the polarization selection rules for different configurations of the scattering experiment. The available data on group-subgroup relations between point and space groups and the corresponding correlations between their irreducible representations permit the analysis of the behaviour of the phonon modes during a symmetry break.

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