

[s14.m40.p1](#) **Bilbao Crystallographic Server: New Database on Layer Groups.** M.I. Aroyo<sup>a</sup>, C. Capillas<sup>a</sup>, P. Konstantinov<sup>b</sup>, J.M. Perez-Mato<sup>a</sup>, H. Wondratschek<sup>c</sup>, <sup>a</sup>*Depto. Física de la Materia Condensada, Universidad del País Vasco, 48080 Bilbao, Spain,* <sup>b</sup>*Institute for Nuclear Research and Nuclear Energy, Bulgarian Academy of Sciences, 1784 Sofia, Bulgaria,* <sup>c</sup>*Institut für Kristallographie, Universität Karlsruhe, 76128 Karlsruhe, Germany* E-mail: [wmparm@lg.ehu.es](mailto:wmparm@lg.ehu.es)

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The Bilbao Crystallographic Server is a web site with crystallographic databases and programs made available worldwide via Internet ([www.cryst.ehu.es](http://www.cryst.ehu.es)) [1]. The core of the server consists of a set of databases including the space-group data of International Tables for Crystallography, Vol. A (abbreviated ITA) [2], the volume on Maximal Subgroups of Plane and Space Groups (abbreviated ITA1) [3], and symmetry properties of reciprocal space (**k**-vector types and Brillouin zones).

The aim of the contribution is to announce the development of a database for the 80 layer groups including generators, general and special positions [4, 5]. The structure of this database is similar to the ITA one, where the basic crystallographic data of the 230 space groups are stored. In addition, the complete information on maximal subgroups of layer groups is made available (similar to the ITA1 database) [6]. All maximal subgroups of index 2, 3 and 4 are listed individually whereas the infinitely many maximal isotypic subgroups are presented as infinite series. For each subgroup either its General position or a set of generators is given. The conjugacy relations of the subgroups in the original group are indicated. The transformation to the conventional coordinate system of the subgroup is available as a matrix for the change of basis and a column for the origin shift. The symmetry information has been stored in a provisional CIF-format. For the extension of the existing CIF-core dictionary a list of data names has been developed which refer to the specific requirements of the subgroup tables of the layer groups. The Bilbao Crystallographic Server provides a free online access to these data.

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**Keywords: Crystal physics; Z. Gyulai; I. Tarján**

"Hungarian Crystallography" was published in 1776 [1]. That book contained 222 figures illustrating crystals found in Hungary, it referred to some physical properties (in most cases to the colour) of the crystals too. The crystal physics in Hungary remained the part of the mineralogical crystallography until the twenties of the last century.

The colour centres in alkali-halogenide crystals was the subject of Z. Gyulai's investigation in his study tour in Göttingen from 1924 to 1926. After returning home at the Szeged University in 1928 he (together with D. Hartly) did his world famous experiment. He unilaterally compressed common salt crystals and observed an increased electrical conductivity in the crystals [2]. Gyulai interpreted the effect by supposing defects in the crystal structure, which was generally thought that time in the light of the success of the X-ray diffraction to be perfectly ideal. ("The first evidence of the formation of point defects by plastic deformation." - as written by F.R.N.Nabarro). Gyulai's experiment has been several times repeated and his paper is cited up to now.

In 1950 Gyulai together with I. Tarján grew quartz crystals of several centimetres by hydrothermal method.

In the early fifties (for the first time in the world) Gyulai measured the tensile strength of whiskers (filamentary crystals). He obtained values, which are of the same order of magnitude as the theoretical value for ideally perfect crystals [3]. Now the whiskers are used in the technology. Twisted NaCl whiskers were observed by Gyulai and E. Hartmann determined the Burgers vector of the screw dislocation in them [4].

I. Tarján arranged for Hungary to join the IUCr in 1963.

The paper about the growth of alkali halide crystals of high purity ( $<10^{-7}$  mol/mol) was the most cited one in the journal where it was published [5]. The Hungarian crystal growers wrote the book [6], "which should be in the hands of all teachers and students of crystal growth" according to C.W. Bunn. The pamphlet "An Introduction to Crystal Physics" (1984, 1998) was written by E. Hartmann for the Teaching Commission of IUCr.

From 1998 the centre of the oxide crystal growth and characterization in Hungary is the Research Institute for Solid State Physics and Optics of the Hungarian Academy of Sciences.

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