## International Tables for Crystallography, Volume A1

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The list of the maximal subgroups of the space groups in Volume A is incomplete. Volume A1 [1] now contains the complete data. Its Part 1 deals with group-theoretical aspects of space groups, group-subgroup relations and the underlying mathematical background. Part 2 contains complete listings of all maximal subgroups for each space group, including their general positions or their generators, their conjugacy relations and transformations to conventional settings. Part 3 lists the relations between the Wyckoff positions for every maximal subgroup of every space group, including the cell transformations and coordinate transformations. In both parts the infinitely many isomorphic subgroups have been included in a parametrized form.

The importance of listing all subgroups individually, not just their types, can be seen in the relations of the AlB<sub>2</sub> structure (*P6/mmm*) with those of ZrBeSi and CaIn<sub>2</sub> which crystallize in two *different* subgroups  $P6_3/mmc$ . The occupied atomic positions of AlB<sub>2</sub> split in different ways to the positions of the two subgroups [2].

The index of symmetry reduction to a maximal isomorphic subgroup may adopt an infinity of values, e.g. p = prime = 6n+1 for certain isomorphic subgroups of  $R\overline{3}$ . Such values are actually being observed, e.g. p = 31 for PtCl<sub>3</sub> [3] as a hettotype of fcc packing. The necessary information for such relations is contained in Volume A1.

[1] International Tables for Crystallography, Vol. A1, 2004, Dordrecht: Kluwer. [2] Hoffmann R.-D., Pöttgen R., Z. Kristallogr. 2001, **216**, 127. [3] Müller U., Z. Anorg. Allg. Chem., 2004, **630**, 1519.

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