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Space-group scanning tables

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Owing to page limitations, in Volume E: *Subperiodic Groups* of *International Tables for Crystallography* not all scanning tables were explicitly given. Instead, auxiliary tables were given providing information from which to construct the additional tables. The tables have been constructed and are presented here.

1. Introduction

If a crystal of a given space-group symmetry is transected by a plane of a crystallographic orientation, *i.e.* an orientation given by integer Miller or Miller–Bravais indices, the subgroup of all elements of the space group that leaves the plane invariant is a layer group. These layer groups, and references to applications in the study of layer symmetries in crystals, interfaces in crystalline materials, and the symmetry of domain twins and domain walls, for all planes of a crystallographic orientation and all space groups, are tabulated in the *scanning tables* of Volume E: *Subperiodic Groups* (*International Tables for Crystallography*, 2002, abbreviated here as ITC:E).

Explicit tables are given for all triclinic and monoclinic space groups. For all other space groups, explicit tables are given only for orientations of planes with *fixed* values of Miller or Miller–Bravais indices, where a single set of indices represents a single planar orientation. For these other space groups and orientations of planes with *variable* values of Miller or Miller–Bravais indices, where a single set of indices represents a set of planar orientations, instructions are provided to construct scanning tables using auxiliary tables.

2. Additional explicit scanning tables

We have constructed from the auxiliary tables explicit scanning tables for the orientations of planes with variable values for all non-triclinic/non-monoclinic space groups.[1] In Table 1, for the space group *Pmm*2, we give an example of an additional explicit scanning table. Details of the structure of scanning tables are given in Part 5.2 of ITC:E. In brief, see Table 1, 'Orientation orbit' groups the orientations of sets of planes that are related by the elements of the space group. The Miller indices ($mn0$), for example, represent a set of indices with variable values, m and n taking any integer value. The 'Scanning group' is the equitranslational subgroup of the space group that leaves invariant the orientation of the plane being considered. The conventional basis of the 'Scanning group' is defined in terms of the basis vectors **a**, **b**, **c** of the space group, the integers p and q satisfy the equation $nq + mp = 1$. The basis vectors $\mathbf{a}'$ and $\mathbf{b}'$ leave the considered plane invariant and **d** gives the direction used to define the position of the plane in the crystal. These positions $s\mathbf{d}$ are given in the 'Linear orbit' column, *i.e.* the considered plane passes through the point $O + s\mathbf{d}$, where O is the origin of the space group. The positions are given by a fixed value of s, *e.g.* $0\mathbf{d}$ and $\frac{1}{2}\mathbf{d}$ or a variable value of s, *e.g.* $s\mathbf{d}$, where $0 < s < 1$ except for fixed values previously listed. The positions of planes related by symmetry elements of the scanning group are placed within square brackets. The layer-group symmetry is given in the final column. The numbering is that of the layer group listing in Part 4 of ITC:E.

Table 1
Space group *Pmm*2: example of additional explicit scanning table.

Orientation orbit (hkl)	Conventional basis of the scanning group $\mathbf{a}'$	$\mathbf{b}'$	$\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}$	
($mn0$)	$\mathbf{c}$	$n\mathbf{a} - m\mathbf{b}$	$p\mathbf{a} + q\mathbf{b}$	$P211$	$0\mathbf{d}, \frac{1}{2}\mathbf{d}$	$p211$	L08
($\bar{m}n0$)	$\mathbf{c}$	$n\mathbf{a} + m\mathbf{b}$	$-p\mathbf{a} + q\mathbf{b}$		$[s\mathbf{d}, -s\mathbf{d}]$	$p1$	L01
($0mn$)	$\mathbf{a}$	$n\mathbf{b} - m\mathbf{c}$	$p\mathbf{b} + q\mathbf{c}$	$Pm11$	$s\mathbf{d}$	$pm11$	L11
($0\bar{m}n$)	$\mathbf{a}$	$n\mathbf{b} + m\mathbf{c}$	$-p\mathbf{b} + q\mathbf{c}$				
($n0m$)	$\mathbf{b}$	$n\mathbf{c} - m\mathbf{a}$	$p\mathbf{c} + q\mathbf{a}$	$Pm11$	$s\mathbf{d}$	$pm11$	L11
($n0\bar{m}$)	$\mathbf{b}$	$n\mathbf{c} + m\mathbf{a}$	$-p\mathbf{c} + q\mathbf{a}$				

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[1] A data file containing these tables is available from the IUCr electronic archives (Reference: SH5019). Services for accessing these data are described at the back of the journal.

References

International Tables for Crystallography (2002). Volume E: *Subperiodic Groups*, edited by V. Kopsky & D. B. Litvin. Dordrecht: Kluwer Academic Publishers.