Note: Handouts used in class contain copyright-protected material from the International Tables for Crystallography that cannot be posted on a web site. Viewers are referred to this book, which is available in most scientific libraries.

Handout 5:

Plane group p3 (p94 in *International Tables for Crystallography, Volume A, 1983)*

Plane group p4gm (p93 in *International Tables for Crystallography, Volume A, 1983)*

Space group *P*2 (p106 in *International Tables for Crystallography, Volume A, 1983)*

Space group $P2_1/c$ (p176-7 in *International Tables for Crystallography, Volume A, 1983)*

Space group *Cmma* (p300-1 in *International Tables for Crystallography, Volume A, 1983)*

Handout 5A:

Page 1-3: see http://it.iucr.org/Ab/resources/explanation.pdf

Table 2.4.1, see p15 in *International Tables for Crystallography, Volume A (1983 ed)*

- Hermann-Mauguin symbols consist of
  - A letter indicating the centering of the cell (*P, R, I, F, C*)
  - A set of characters indicating symmetry elements of the space group
- Use lower case letters for plane group centering, capital letters for space group centering
- The one, two or three entries after the centering letter refer to one, two or three kinds of symmetry directions of the lattice as outlined in Table 2.4.1
  - Can be singular directions (monoclinic and orthorhombic) or sets of equivalent directions
- Symmetry planes are represented by their normals
  - If a symmetry axis and a symmetry plane are parallel, the two characters are separated by s slash, e.g. *P*2/*m*
- The symbol 1 is used for lattice directions that carry no symmetry elements
  - These entries can be omitted if no misinterpretation is possible, e.g. *P*6 instead of *P*611 etc.
  - For monoclinic space groups, the full symbol allows to distinguish standard settings (unique axis b) from non-standard settings (unique axis a or c)
  - For high symmetry space groups, symmetry axes are often suppressed in the short symbol (e.g., *Pnma* vs. $P\ 2_1/n\ 2_1/m\ 2_1/a$)
- Letters in space group symbols are placed in italic font, numbers are not.

Space group diagrams

- Show the relative locations and orientations of the symmetry elements
  - Depending on how complex the space group symmetry is, one or several drawings can be used
- Illustrate the arrangement of a set of symmetry equivalent points of a general position
  - A "general position" is any point in the unit cell that does not coincide with any symmetry elements
  - Maximum number of atoms generated
- Except for representations with rhombohedral axes, all projection directions are along a cell axis
  - In rhombohedral, triclinic and monoclinic cells, this can result in the other axes not being parallel to the plane of projection and is indicated by a subscript *p*
- Symmetry elements that lie above the plane of projection are designated by the height *h* above the plane. *h* is given as a fraction along the lattice direction of projection
- For rhombohedral space groups, two settings are given, one with rhombohedral and one with hexagonal axes

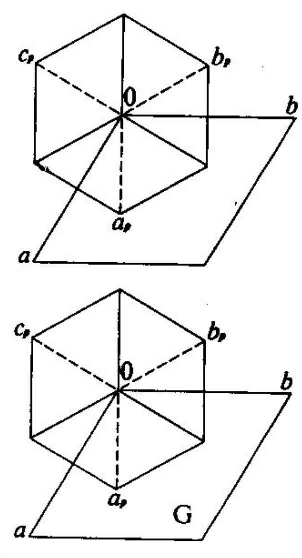

Fig. 2.6.9. Rhombohedral *R* space groups. Obverse triple hexagonal cell with 'hexagonal axes' *a*, *b* and primitive rhombohedral cell with projections of 'rhombohedral axes' a_p, b_p, c_p. Note: In the actual space-group diagrams only the upper edges (full lines), not the lower edges (dashed lines) of the primitive rhombohedral cell are shown (G = General-position diagram).

Choice of origin

- In all centrosymmetric space groups, the origin is chosen on an inversion center
    - A second origin choice can be given if there are other high symmetry sites
- In all non-centrosymmetric space groups, the origin is at the point of highest symmetry
    - Usually the highest rotation axis
    - Screw axes are used if no simple rotation axes are present
    - If no rotation or screw axes are present, the intersection of mirror and glide planes is chosen as origin
    - Exceptions: In $P2_12_12_1$ and related supergroups, the origin is chosen so that it is surrounded symmetrically by three pairs of 2_1 axes

Asymmetric unit

- The smallest part of space from which the whole of space can be filled exactly by application of all symmetry operations
    - Mirror planes and rotation axes must form boundary planes and edges
    - Centers of inversion must be on vertices or at the midpoints of boundary planes or edges
- For higher symmetry unit cells, the shape of the asymmetric unit can be rather complicated

Sub- and supergroups

- Can be used to describe symmetry related space groups
- Subgroups contain a set of symmetry operations that also belongs to the space group being discussed
  - The set of symmetry operations must also form a space group
  - If it is possible to take symmetry elements away "step by step", an "order" of space groups can be established with decreasing symmetry: G > M > H
  - A subgroup H is called a *maximal subgroup* if there is no subgroup of higher symmetry between H and G (example: $P2_1/c$ has $P2_1$, Pc and P-1 as maximal subgroups, while P1 is a non-maximal subgroup)
  - All subgroups can be listed as *chains* of maximal subgroups (e.g., $P2_1/c$ > P-1 > P1)
- Symmetry can be reduced by several means
  - Removal of point symmetry elements: *translationsgleiche* or *t* subgroups (translation equivalent)
  - "Thinning out" of symmetry operations, e.g. doubling of a cell axis in the same space group, which is equivalent to loss of translational symmetry, or by replacing rotation axes by screw axes: *klassengleiche* or *k* subgroups (same class/point group)
- Supergroups are the opposite of subgroups, so if a space group *X* is listed as a subgroup of another space group *Y*, then *Y* must be listed as a supergroup of *X*