Appendix E

Orbit spaces for 3D-irreducible Bravais groups

There are three cubic Bravais groups $Pm\bar{3}m$, $Im\bar{3}m$, $Fm\bar{3}m$, corresponding to the same point symmetry group, O_h. We construct orbifolds for these three-dimensional irreducible Bravais groups to see the difference of group actions.

We start with the $Pm\bar{3}m$ group. Its elementary cell includes one point of the simple cubic lattice and is supposed to be of volume one. We use this primitive cell to represent different strata of the symmetry group action. Different strata (or systems of different Wyckoff positions according to ITC) are shown in Figure E.1.

There are two zero dimensional strata with stabilizer O_h, characterized as Wyckoff position a and b. The stabilizers of these two strata are not conjugate in the symmetry group of the lattice. Points a correspond to points forming the simple cubic lattice. Points b are situated in the center of the cubic cell formed by points a. Eight points of type a are shown in Figure E.1 but as soon as each point equally belongs to eight cells there is only one point a per cell.

There are also two zero-dimensional strata with stabilizer D_{4h} which are not conjugate in the symmetry group of the lattice. They are labeled as c and d (according to ITC). There are three positions of type c per cell and three positions of type d per cell. Each point of type c belongs to two cells whereas each point of type d belongs to 4 cells. That is why there are 6 points of type c and 12 points of type d drawn in Figure E.1.

There are six different one-dimensional strata of the $Pm\bar{3}m$ group action on the space. Two one-dimensional strata have as stabilizers two C_{4v} subgroups which are not conjugate in the lattice symmetry group. These two strata are shown on the same subfigure in Figure E.1. Each orbit of e (solid line) symmetry type has six points per primitive cell. Two points of each orbit are situated on each of three disconnected intervals shown by solid thick line. As soon as these solid lines are edges of the primitive cell and belong, in fact, to four cells, all other edges are equivalent and consequently belong to the

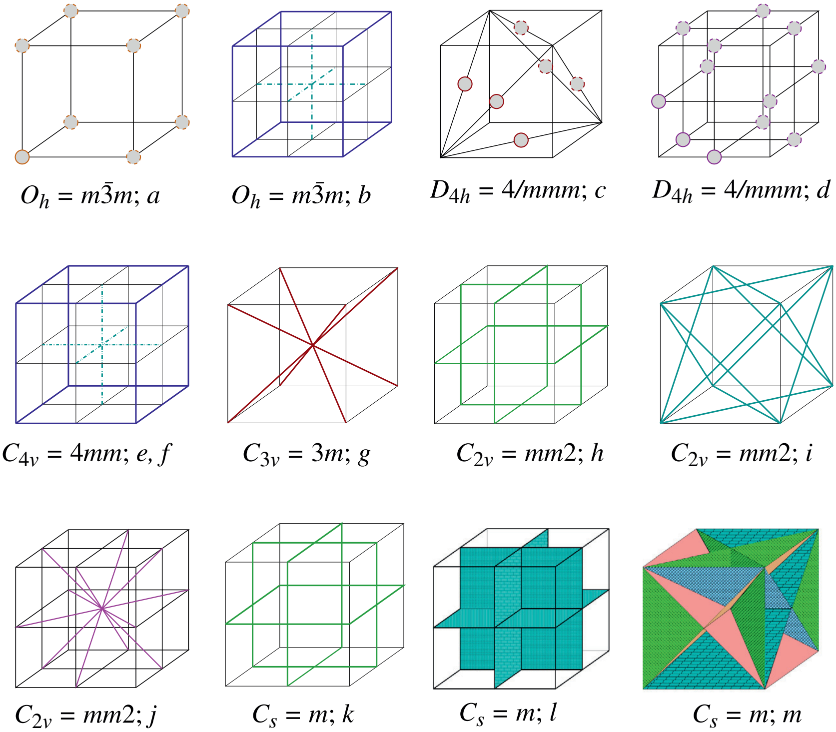

FIG. E.1 – Different strata for $Pm\bar{3}m$ Bravais group.

same stratum. Orbits of f type are situated inside the primitive cell on six intervals marked by the dash-dot line. One point of each orbit belongs to one of six equivalent intervals forming one stratum.

The C_{3v} stratum (type g of Wyckoff positions) consists of orbits having eight points per cell situated on the diagonals of primitive cell.

There are three non-conjugated C_{2v} strata (types h, i, j of Wyckoff positions). These strata are shown in three subfigures of Figure E.1. Each orbits has 12 points per cell for each of these three strata.

There are also three two-dimensional strata k, l, m. Each of them has $C_s \equiv m$ group as the stabilizer, but all of these three stabilizers are non-conjugate subgroups of the lattice symmetry group. The last three subfigures of E.1 show these strata. (Better visualization of m stratum can be done by using three rather than one subfigures. This is done for the $Fm\bar{3}m$ group in figure E.7, see three initial figures for stratum k.) Each orbit belonging to these strata has 24 points per cell.

At last, all points which do not belong to the mentioned above strata form generic stratum with trivial stabilizer $1 \equiv C_1$. It consists of orbits having 48 points per cell.

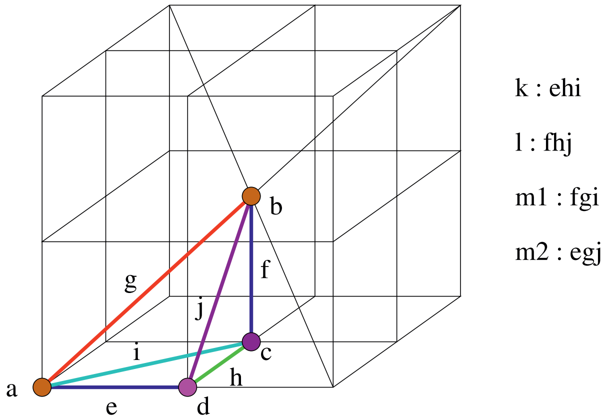

FIG. E.2 – Primitive cell and orbifold for the $Pm\bar{3}m$ three-dimensional Bravais group.

In order to construct the orbifold of the $Pm\bar{3}m$ group action we can choose a closed region (simplex) shown in Figure E.2. Its vertices are points from different zero-dimensional strata a, b, c, d. Six of its edges are also formed by points belonging to different one-dimensional strata: $e : a - d$; $f : b - c$; $g : a - b$; $h : c - d$; $i : a - c$; $j : b - d$. (Each edge is indicated by its two boundary vertices.) Among four faces, two belong to the same stratum of type m, namely, $m1 : fgi$ and $m2 : egj$ (the face is indicated by its three boundary edges). Each of two other faces belongs to its proper stratum: $k : ehi$, $l : fhj$. Internal points belong to generic stratum, n.

Topologically, the orbifold of the $Pm\bar{3}m$ group is a three-dimensional disk with all internal points belonging to the generic stratum and the boundary formed by 13 different strata.

Now we turn to the $Im\bar{3}m$ Bravais group. In order to have a cell whose symmetry coincides with the symmetry of the lattice, we are obliged to take a double cell which has volume 2 and includes two lattice points per cell. Different strata of the $Im\bar{3}m$ action are shown in Figure E.3. It is instructive to briefly compare the system of strata of $Im\bar{3}m$ with that of $Pm\bar{3}m$ by ignoring the difference in volumes of cells. The notation of strata by Latin letters follows again the notation of Wyckoff positions in ITC. Zero dimensional stratum a (stabilizer O_h) of $Im\bar{3}m$ includes points of strata a and b of $Pm\bar{3}m$. Zero dimensional stratum b of $Im\bar{3}m$ (stabilizer D_{4h}) includes points of strata c and d of $Pm\bar{3}m$. Zero dimensional strata c (stabilizer D_{3d}) and d (stabilizer D_{2d}) of $Im\bar{3}m$ are the new ones as compared to stratification imposed by $Pm\bar{3}m$.

One-dimensional stratum e of $Im\bar{3}m$ includes points belonging to e and f strata of $Pm\bar{3}m$. Stratum f (stabilizer C_{3v}) of $Im\bar{3}m$ action coincides with the stratum g of $Pm\bar{3}m$. The group $Im\bar{3}m$ has three one-dimensional strata

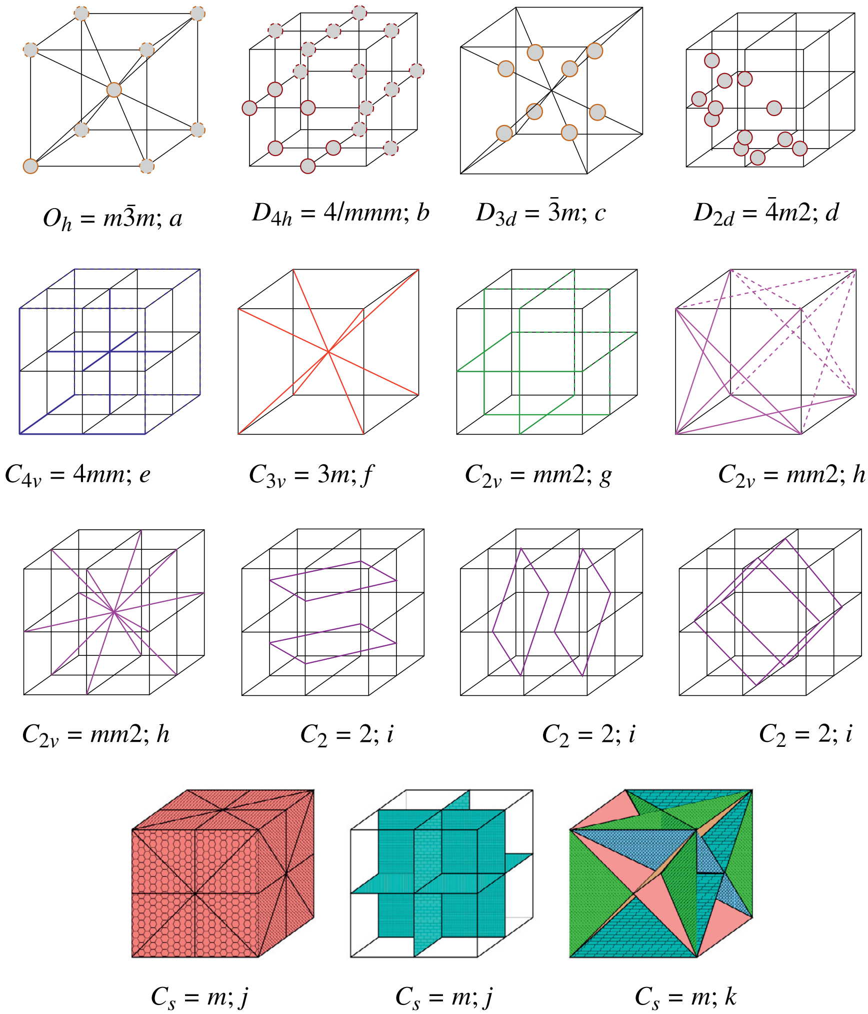

FIG. E.3 – Different strata for the $Im\bar{3}m$ Bravais group. In order to simplify visualization of the stratum d with stabilizer D_{2d} only translationally inequivalent points are represented.

g, h, i with stabilizer C_{2v}. The one-dimensional stratum g of $Im\bar{3}m$ action coincides with stratum h of $Pm\bar{3}m$. The one-dimensional stratum h of $Im\bar{3}m$ includes points of two strata i and j of $Pm\bar{3}m$. The one-dimensional stratum i of $Im\bar{3}m$ is a new one as compared to the stratification imposed by $Pm\bar{3}m$.

The two-dimensional stratum j (stabilizer C_s) of $Im\bar{3}m$ includes points belonging to two strata k and l of $Pm\bar{3}m$. The two-dimensional stratum k (stabilizer C_s) of $Im\bar{3}m$ reproduces stratum m of $Pm\bar{3}m$.

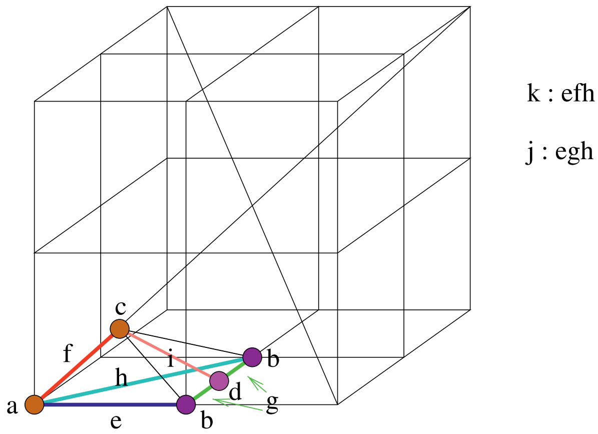

FIG. E.4 – Double cell and orbifold for the $Im\bar{3}m$ three-dimensional Bravais group.

In order to construct the orbifold and to take only one point from each orbit we can take the region shown in Figure E.4. The choice of this region coincides with the choice of the asymmetric unit suggested by ITC for the $Im\bar{3}m$ group. One should only additionally take into account the following important facts.

i) The two points marked by b in E.4 belong to the same stratum b and moreover to the same orbit with stabilizer D_{4h}. This can be easily seen because all points on the line cd have stabilizer C_2 and this C_2 rotation is obviously rotation around the cd line. This C_2 symmetry transformation unifies not only two points marked b into one orbit but also it acts on any point of the bcb triangular face of the chosen region. This indicates that pairs of respective points in two cbd triangles should be identified in order to construct the orbifold including only one point from each orbit. From the topological point of view the result of gluing two cbd triangles is the orbifold shown in Figure E.5. It can be represented as a three-dimensional body having the geometrical form of a double cone with two special points (c, d) at its apexes and two special points (a, b) on the equator. Moreover, all other points of the equator belong to two different (h and e) one-dimensional strata. Two other one-dimensional strata connect on the surface of double cone points a and c (stratum f) and points b and d (stratum g). Inside a double cone there is one more one-dimensional stratum i connecting points c and d. All other internal points belong to generic stratum l. Boundary points of the double cone which do not belong to the mentioned above zero-dimensional and one-dimensional strata form two two-dimensional strata. Stratum k consists of points of the upper part of the double cone boundary. This two-dimensional stratum has one-dimensional strata f, h, and e as its boundary. Stratum j consists of

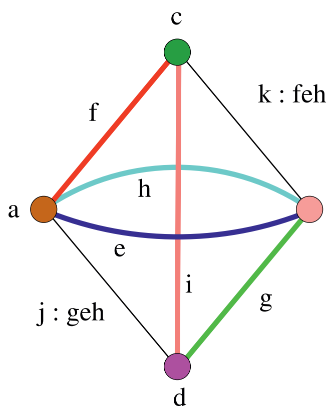

FIG. E.5 – Schematic representation of the orbifold for the $Im\bar{3}m$ three-dimensional Bravais group.

points of the lower part of the double cone boundary. This two-dimensional stratum has one-dimensional strata g, e, and h as its boundary.

In the case of the $Fm\bar{3}m$ Bravais group the choice of the cell respecting the O_h holohedry of the lattice leads to the quadruple cell of volume 4 as compared to the primitive cell. All zero-, one- and two-dimensional strata of the lattice symmetry group action on this quadruple cell are shown in Figures E.6, E.7.

The notation of strata by Latin letters follows again the notation of Wyckoff positions adapted in ITC. A zero dimensional stratum with stabilizer D_{2d} is shown in two subfigures in order to see better the location of all points. In this case one orbit includes 24 points per quadruple cell. In a similar way a one-dimensional stratum of type f (stabilizer C_{3v}) is represented in four sub-figures. Two of three non-conjugated in the lattice symmetry group strata with stabilizer C_{2v}, namely strata of type h and i, are also shown in two sub-figures. A two-dimensional stratum of type j (stabilizer C_s) is represented in two subfigures which coincide with figures of stratum j of Bravais group $Im\bar{3}m$. A two-dimensional stratum of type k (stabilizer C_s) is represented in six subfigures. Three of these subfigures reproduce figures of stratum k for the $Im\bar{3}m$ group or stratum m for the $Pm\bar{3}m$ group.

In order to construct the orbifold we need to take one representative point from each orbit. This can be done by restricting the quadruple cell to the region having tetrahedral geometry (see figure E.8) with coordinates of vertices
$a : \{0, 0, 0\}$; $b : \{1/2, 0, 0\}$; $c : \{1/4, 1/4, 1/4\}$; $d : \{1/4, 1/4, 0\}$.

This choice coincides with the choice of the asymmetric unit for the $Fm\bar{3}m$ group made in ITC. The $Fm\bar{3}m$ orbifold is a topological three-dimensional disk. All its internal points belong to the generic C_1 stratum. The stratification

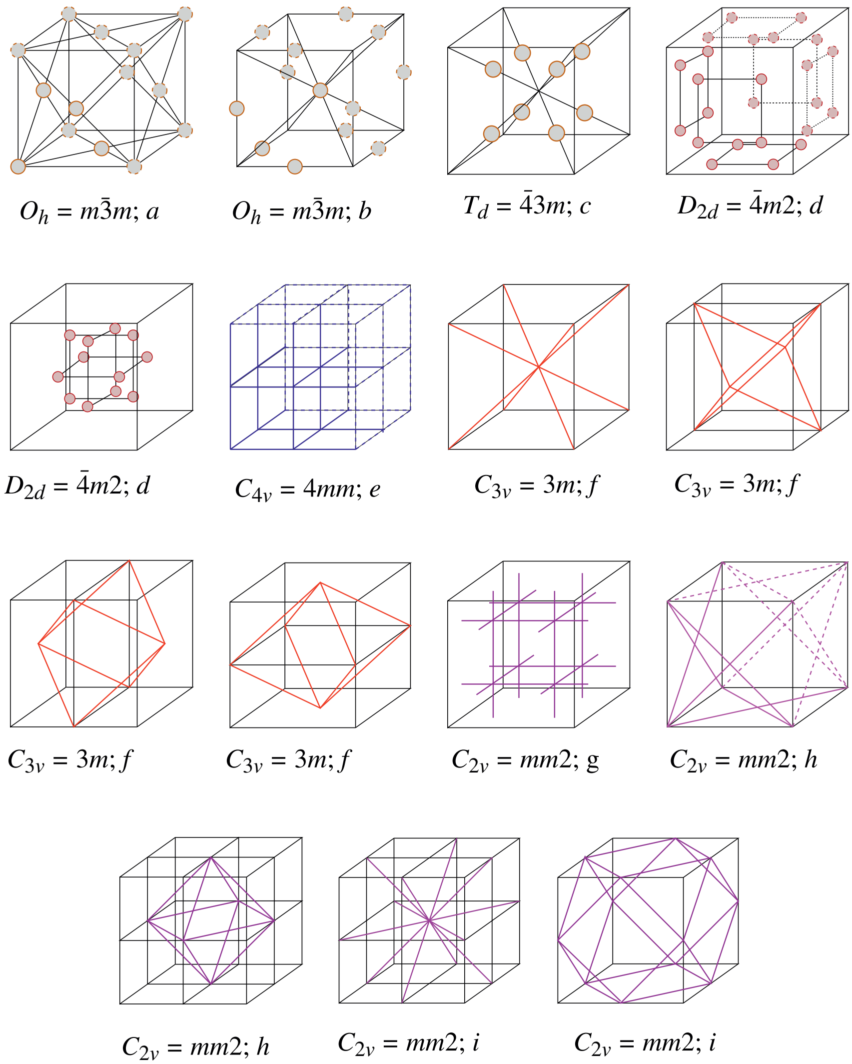

FIG. E.6 – Different zero- and one-dimensional strata for the $Fm\bar{3}m$ Bravais group.

of boundary is similar to the $Pm\bar{3}m$ orbifold. For $Fm\bar{3}m$ all four vertices belong to different zero-dimensional strata, but among six edges there are two belonging to the same stratum, and among four faces, three belong to the same stratum.

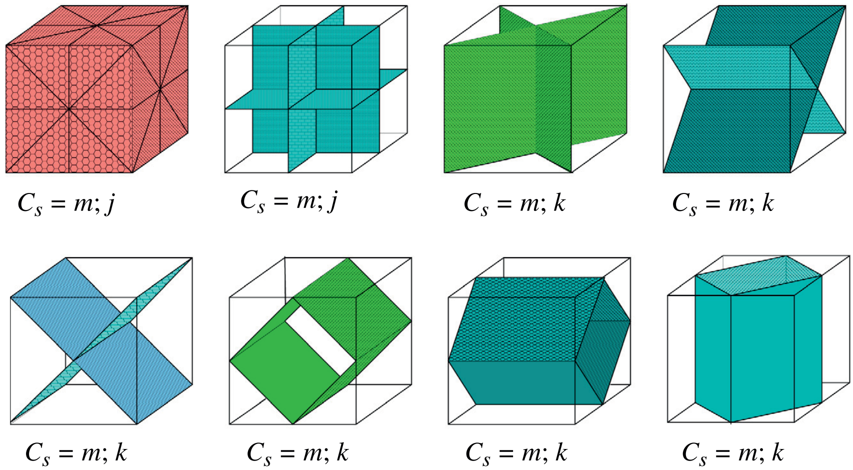

FIG. E.7 – Different two-dimensional strata for the $Fm\bar{3}m$ Bravais group.

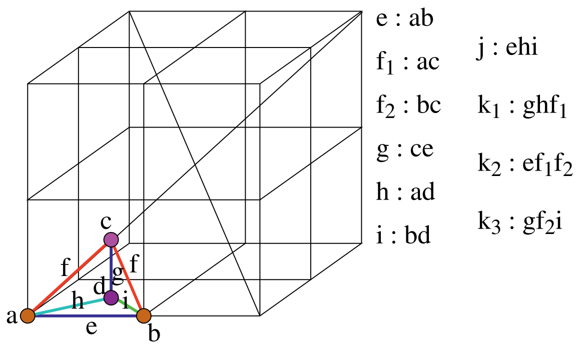

FIG. E.8 – Schematic representation of orbifold for the $Fm\bar{3}m$ three-dimensional Bravais group.