For specific space group, the whole lattice structure should be deduced according to the symmetric operation (elements of corresponding space group). The basis for above stuff is that the fractional coordinates of every atom in asymmetric unit has been given. The deduction process is that for each atomic position in the asymmetric unit, the ‘deduced’ position can be obtained following the symmetric operation (specified for each space group). However, it is not every atomic position in the asymmetric unit can distinctively create new positions following the space group elements one by one, for example, if an atom stays at (0.2, 0, 0.2) in the lattice structure with Pm space group symmetric properties (mirror plane perpendicular to b axis), the mirror reflection operation belonging to this space group will not create new position (the position coordinate it creates is the same with the starting coordinate), this kind of position is called **Special Position**, and the other positions are called **General Position (s)**. The number of distinct positions corresponding to one definite atomic position within specific space group is called **Multiplicity**. In fact, there will always be many atomic positions with the same multiplicity within one space group. This kind of positions is classified as a group for which a specific letter is given, and this kind of positions’ group is called **Wyckoff Site**. The letter is alphabetically decided by multiplicity of **Wyckoff Sites**, the bigger the multiplicity is, the latter the letter lays. For example, ‘96k’ **Wyckoff Site** belongs to the space group of ‘F m -3 m’ has the multiplicity of 96 and Wyckoff letter of ‘k’.

Given the specific space group and atomic fractional coordinate for each atom within the motif, all the positions of each atom can be deduced according to the classification of Wyckoff Sites. Taking the following table (Wyckoff Sites of space group ‘Fm-3m’) as an example, given the atomic fractional coordinate, the first step is to look up which Wyckoff site this position belongs to. Having settled in specific Wyckoff Site, the next step is to rewrite the coordinates according to the form of all the elements within this Wyckoff Site, e. g. for (0.2, 0.2, 0.2) belonging to ‘32f’, the following coordinates should be written down:

(-0.2, -0.2, 0.2), (0.2, -0.2, -0.2), (-0.2, 0.2, -0.2), (-0.2, -0.2, -0.2), (0.2, 0.2, -0.2), (0.2, -0.2, 0.2), (-0.2, 0.2, 0.2), (0.2, 0.2, 0.2)

For each site belonging to the same Wyckoff Site, the new coordinates are always the same, which is another way to understand why these coordinates are in the same **Wyckoff Site**.

The last step is to consider the combination of **space group generators** **(operators within the labelled region of the following table)** and **Wyckoff Site**, so in this case, for each atomic position given, there should be four series of coordinates to be deduced. Here, the **space group generators** refer to the atomic position determined by the space group in a single lattice cell.

For more information and all the **Wyckoff Sites** tables, just Google ‘**Wyckoff Site**’

**Wyckoff Positions of Group 225 (*Fm*-3*m*)**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Multiplicity** | **Wyckoff letter** | **Site symmetry** | **Coordinates** | |
| (0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) + |  |
| 192 | l | 1 | |  |  |  |  | | --- | --- | --- | --- | | [(x,y,z)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=x&yc=y&zc=z&orgpos=x,y,z&standard=1) | [(-x,-y,z)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=-x&yc=-y&zc=z&orgpos=-x,-y,z&standard=1) | [(-x,y,-z)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=-x&yc=y&zc=-z&orgpos=-x,y,-z&standard=1) | [(x,-y,-z)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=x&yc=-y&zc=-z&orgpos=x,-y,-z&standard=1) | | [(z,x,y)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=z&yc=x&zc=y&orgpos=z,x,y&standard=1) | [(z,-x,-y)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=z&yc=-x&zc=-y&orgpos=z,-x,-y&standard=1) | [(-z,-x,y)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=-z&yc=-x&zc=y&orgpos=-z,-x,y&standard=1) | 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| 96 | k | ..m | |  |  |  |  | | --- | --- | --- | --- | | [(x,x,z)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=x&yc=x&zc=z&orgpos=x,x,z&standard=1) | [(-x,-x,z)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=-x&yc=-x&zc=z&orgpos=-x,-x,z&standard=1) | [(-x,x,-z)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=-x&yc=x&zc=-z&orgpos=-x,x,-z&standard=1) | [(x,-x,-z)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=x&yc=-x&zc=-z&orgpos=x,-x,-z&standard=1) | | [(z,x,x)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=z&yc=x&zc=x&orgpos=z,x,x&standard=1) | [(z,-x,-x)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=z&yc=-x&zc=-x&orgpos=z,-x,-x&standard=1) | [(-z,-x,x)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=-z&yc=-x&zc=x&orgpos=-z,-x,x&standard=1) | [(-z,x,-x)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=-z&yc=x&zc=-x&orgpos=-z,x,-x&standard=1) | | [(x,z,x)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=x&yc=z&zc=x&orgpos=x,z,x&standard=1) | [(-x,z,-x)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=-x&yc=z&zc=-x&orgpos=-x,z,-x&standard=1) | [(x,-z,-x)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=x&yc=-z&zc=-x&orgpos=x,-z,-x&standard=1) | [(-x,-z,x)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=-x&yc=-z&zc=x&orgpos=-x,-z,x&standard=1) | | [(x,x,-z)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=x&yc=x&zc=-z&orgpos=x,x,-z&standard=1) | [(-x,-x,-z)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=-x&yc=-x&zc=-z&orgpos=-x,-x,-z&standard=1) | [(x,-x,z)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=x&yc=-x&zc=z&orgpos=x,-x,z&standard=1) | [(-x,x,z)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=-x&yc=x&zc=z&orgpos=-x,x,z&standard=1) | | [(x,z,-x)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=x&yc=z&zc=-x&orgpos=x,z,-x&standard=1) | [(-x,z,x)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=-x&yc=z&zc=x&orgpos=-x,z,x&standard=1) | [(-x,-z,-x)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=-x&yc=-z&zc=-x&orgpos=-x,-z,-x&standard=1) | [(x,-z,x)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=x&yc=-z&zc=x&orgpos=x,-z,x&standard=1) | | [(z,x,-x)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=z&yc=x&zc=-x&orgpos=z,x,-x&standard=1) | [(z,-x,x)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=z&yc=-x&zc=x&orgpos=z,-x,x&standard=1) | [(-z,x,x)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=-z&yc=x&zc=x&orgpos=-z,x,x&standard=1) | [(-z,-x,-x)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=-z&yc=-x&zc=-x&orgpos=-z,-x,-x&standard=1) | |  |
| 96 | j | m.. | |  |  |  |  | | --- | --- | --- | --- | | [(0,y,z)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=0&yc=y&zc=z&orgpos=0,y,z&standard=1) | [(0,-y,z)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=0&yc=-y&zc=z&orgpos=0,-y,z&standard=1) | [(0,y,-z)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=0&yc=y&zc=-z&orgpos=0,y,-z&standard=1) | [(0,-y,-z)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=0&yc=-y&zc=-z&orgpos=0,-y,-z&standard=1) | | [(z,0,y)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=z&yc=0&zc=y&orgpos=z,0,y&standard=1) | [(z,0,-y)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=z&yc=0&zc=-y&orgpos=z,0,-y&standard=1) | [(-z,0,y)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=-z&yc=0&zc=y&orgpos=-z,0,y&standard=1) | [(-z,0,-y)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=-z&yc=0&zc=-y&orgpos=-z,0,-y&standard=1) | | [(y,z,0)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=y&yc=z&zc=0&orgpos=y,z,0&standard=1) | [(-y,z,0)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=-y&yc=z&zc=0&orgpos=-y,z,0&standard=1) | [(y,-z,0)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=y&yc=-z&zc=0&orgpos=y,-z,0&standard=1) | [(-y,-z,0)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=-y&yc=-z&zc=0&orgpos=-y,-z,0&standard=1) | | [(y,0,-z)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=y&yc=0&zc=-z&orgpos=y,0,-z&standard=1) | [(-y,0,-z)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=-y&yc=0&zc=-z&orgpos=-y,0,-z&standard=1) | [(y,0,z)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=y&yc=0&zc=z&orgpos=y,0,z&standard=1) | [(-y,0,z)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=-y&yc=0&zc=z&orgpos=-y,0,z&standard=1) | | [(0,z,-y)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=0&yc=z&zc=-y&orgpos=0,z,-y&standard=1) | [(0,z,y)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=0&yc=z&zc=y&orgpos=0,z,y&standard=1) | [(0,-z,-y)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=0&yc=-z&zc=-y&orgpos=0,-z,-y&standard=1) | [(0,-z,y)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=0&yc=-z&zc=y&orgpos=0,-z,y&standard=1) | | [(z,y,0)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=z&yc=y&zc=0&orgpos=z,y,0&standard=1) | [(z,-y,0)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=z&yc=-y&zc=0&orgpos=z,-y,0&standard=1) | [(-z,y,0)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=-z&yc=y&zc=0&orgpos=-z,y,0&standard=1) | [(-z,-y,0)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=-z&yc=-y&zc=0&orgpos=-z,-y,0&standard=1) | |  |
| 48 | i | m.m 2 | |  |  |  |  | | --- | --- | --- | --- | | [(1/2,y,y)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=1/2&yc=y&zc=y&orgpos=1/2,y,y&standard=1) | [(1/2,-y,y)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=1/2&yc=-y&zc=y&orgpos=1/2,-y,y&standard=1) | [(1/2,y,-y)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=1/2&yc=y&zc=-y&orgpos=1/2,y,-y&standard=1) | [(1/2,-y,-y)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=1/2&yc=-y&zc=-y&orgpos=1/2,-y,-y&standard=1) | | [(y,1/2,y)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=y&yc=1/2&zc=y&orgpos=y,1/2,y&standard=1) | [(y,1/2,-y)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=y&yc=1/2&zc=-y&orgpos=y,1/2,-y&standard=1) | [(-y,1/2,y)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=-y&yc=1/2&zc=y&orgpos=-y,1/2,y&standard=1) | [(-y,1/2,-y)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=-y&yc=1/2&zc=-y&orgpos=-y,1/2,-y&standard=1) | | [(y,y,1/2)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=y&yc=y&zc=1/2&orgpos=y,y,1/2&standard=1) | [(-y,y,1/2)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=-y&yc=y&zc=1/2&orgpos=-y,y,1/2&standard=1) | [(y,-y,1/2)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=y&yc=-y&zc=1/2&orgpos=y,-y,1/2&standard=1) | [(-y,-y,1/2)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=-y&yc=-y&zc=1/2&orgpos=-y,-y,1/2&standard=1) | |  |
| 48 | h | m.m 2 | |  |  |  |  | | --- | --- | --- | --- | | [(0,y,y)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=0&yc=y&zc=y&orgpos=0,y,y&standard=1) | [(0,-y,y)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=0&yc=-y&zc=y&orgpos=0,-y,y&standard=1) | [(0,y,-y)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=0&yc=y&zc=-y&orgpos=0,y,-y&standard=1) | [(0,-y,-y)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=0&yc=-y&zc=-y&orgpos=0,-y,-y&standard=1) | | [(y,0,y)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=y&yc=0&zc=y&orgpos=y,0,y&standard=1) | [(y,0,-y)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=y&yc=0&zc=-y&orgpos=y,0,-y&standard=1) | [(-y,0,y)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=-y&yc=0&zc=y&orgpos=-y,0,y&standard=1) | [(-y,0,-y)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=-y&yc=0&zc=-y&orgpos=-y,0,-y&standard=1) | | [(y,y,0)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=y&yc=y&zc=0&orgpos=y,y,0&standard=1) | [(-y,y,0)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=-y&yc=y&zc=0&orgpos=-y,y,0&standard=1) | [(y,-y,0)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=y&yc=-y&zc=0&orgpos=y,-y,0&standard=1) | [(-y,-y,0)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=-y&yc=-y&zc=0&orgpos=-y,-y,0&standard=1) | |  |
| 48 | g | 2.m m | |  |  |  |  | | --- | --- | --- | --- | | [(x,1/4,1/4)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=x&yc=1/4&zc=1/4&orgpos=x,1/4,1/4&standard=1) | [(-x,3/4,1/4)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=-x&yc=3/4&zc=1/4&orgpos=-x,3/4,1/4&standard=1) | [(1/4,x,1/4)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=1/4&yc=x&zc=1/4&orgpos=1/4,x,1/4&standard=1) | [(1/4,-x,3/4)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=1/4&yc=-x&zc=3/4&orgpos=1/4,-x,3/4&standard=1) | | [(1/4,1/4,x)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=1/4&yc=1/4&zc=x&orgpos=1/4,1/4,x&standard=1) | [(3/4,1/4,-x)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=3/4&yc=1/4&zc=-x&orgpos=3/4,1/4,-x&standard=1) | [(1/4,x,3/4)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=1/4&yc=x&zc=3/4&orgpos=1/4,x,3/4&standard=1) | [(3/4,-x,3/4)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=3/4&yc=-x&zc=3/4&orgpos=3/4,-x,3/4&standard=1) | | [(x,1/4,3/4)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=x&yc=1/4&zc=3/4&orgpos=x,1/4,3/4&standard=1) | [(-x,1/4,1/4)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=-x&yc=1/4&zc=1/4&orgpos=-x,1/4,1/4&standard=1) | [(1/4,1/4,-x)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=1/4&yc=1/4&zc=-x&orgpos=1/4,1/4,-x&standard=1) | [(1/4,3/4,x)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=1/4&yc=3/4&zc=x&orgpos=1/4,3/4,x&standard=1) | |  |
| 32 | f | .3m | |  |  |  |  | | --- | --- | --- | --- | | [(x,x,x)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=x&yc=x&zc=x&orgpos=x,x,x&standard=1) | [(-x,-x,x)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=-x&yc=-x&zc=x&orgpos=-x,-x,x&standard=1) | [(-x,x,-x)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=-x&yc=x&zc=-x&orgpos=-x,x,-x&standard=1) | [(x,-x,-x)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=x&yc=-x&zc=-x&orgpos=x,-x,-x&standard=1) | | [(x,x,-x)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=x&yc=x&zc=-x&orgpos=x,x,-x&standard=1) | [(-x,-x,-x)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=-x&yc=-x&zc=-x&orgpos=-x,-x,-x&standard=1) | [(x,-x,x)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=x&yc=-x&zc=x&orgpos=x,-x,x&standard=1) | [(-x,x,x)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=-x&yc=x&zc=x&orgpos=-x,x,x&standard=1) | |  |
| 24 | e | 4m. m | |  |  |  |  | | --- | --- | --- | --- | | [(x,0,0)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=x&yc=0&zc=0&orgpos=x,0,0&standard=1) | [(-x,0,0)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=-x&yc=0&zc=0&orgpos=-x,0,0&standard=1) | [(0,x,0)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=0&yc=x&zc=0&orgpos=0,x,0&standard=1) | [(0,-x,0)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=0&yc=-x&zc=0&orgpos=0,-x,0&standard=1) | | [(0,0,x)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=0&yc=0&zc=x&orgpos=0,0,x&standard=1) | [(0,0,-x)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=0&yc=0&zc=-x&orgpos=0,0,-x&standard=1) |  |  | |  |
| 24 | d | m.m m | |  |  |  |  | | --- | --- | --- | --- | | [(0,1/4,1/4)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=0&yc=1/4&zc=1/4&orgpos=0,1/4,1/4&standard=1) | [(0,3/4,1/4)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=0&yc=3/4&zc=1/4&orgpos=0,3/4,1/4&standard=1) | [(1/4,0,1/4)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=1/4&yc=0&zc=1/4&orgpos=1/4,0,1/4&standard=1) | [(1/4,0,3/4)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=1/4&yc=0&zc=3/4&orgpos=1/4,0,3/4&standard=1) | | [(1/4,1/4,0)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=1/4&yc=1/4&zc=0&orgpos=1/4,1/4,0&standard=1) | [(3/4,1/4,0)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=3/4&yc=1/4&zc=0&orgpos=3/4,1/4,0&standard=1) |  |  | |  |
| 8 | c | -43m | |  |  | | --- | --- | | [(1/4,1/4,1/4)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=1/4&yc=1/4&zc=1/4&orgpos=1/4,1/4,1/4&standard=1) | [(1/4,1/4,3/4)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=1/4&yc=1/4&zc=3/4&orgpos=1/4,1/4,3/4&standard=1) | |  |
| 4 | b | m-3m | |  | | --- | | [(1/2,1/2,1/2)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=1/2&yc=1/2&zc=1/2&orgpos=1/2,1/2,1/2&standard=1) | |  |
| 4 | a | m-3m | |  | | --- | | [(0,0,0)](http://www.cryst.ehu.es/cgi-bin/cryst/programs/find_comp_op?ita=225&xc=0&yc=0&zc=0&orgpos=0,0,0&standard=1) | |  |