

1.114: Wyckoff position

A **Wyckoff position** of a space group G consists of all points X for which the site-symmetry groups are conjugate subgroups of G .

Each Wyckoff position of a space group is labeled by a letter which is called the *Wyckoff letter*.

The number of different Wyckoff positions of each space group is finite, the maximal numbers being 9 for plane groups (realized in $p2mm$) and 27 for space groups (realized in $Pmmm$).

There is a total of 72 Wyckoff positions in plane groups and 1731 Wyckoff positions in space groups.

The transfer of Wyckoff positions from individual space groups to space-group types is not unique because Wyckoff positions with the same type of site-symmetry group may be exchanged in different space groups of the same type. This is no longer true when one makes use of Wyckoff sets.

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