

Characterization of Structure Types by Lattice Complexes with Increased Self-Coordination Numbers

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Most of the 402 characteristic Wyckoff positions were analyzed for the numbers 1, 2, 3, etc. of lattice complexes with increased self-coordination numbers T_i of the $i = 1 - 3$ shells. The Wyckoff letters of standardized inorganic structures with the proper space group number get an additional number 1, 2, 3, etc., if the x , y , z , c/a , $\cos \gamma$, etc. parameters are close to the parameters of these lattice complexes. The lattice complexes 1, 2, 3, etc. or combinations of several of these complexes are sphere, layer or rod packings. The plate- or needle-like habit of single crystals can frequently be correlated with layered or rod-like packings. Combinations of lattice complexes can be analyzed for attractive or repulsive interactions by structure maps.

Key words: Wyckoff Sequence, Characteristic Lattice Complexes, Crystal Habit, Sphere Packings, Structure Map