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Highly Regular Spatial Structures: Theory, Software, and Visualization

The mathematical study of highly regular spatial structures has obvious implications in the molecular sciences. As it turns out, a combinatorial version of orbifold theory – the theory of Delaney symbols – can be used very efficiently here.

Regarding 3D-tilings related to crystall structure, several classification problems could be solved in this way: e. g., there are exactly 9 topologically distinct tilings of euclidean 3-space by symmetry-equivalent tetrahedral tiles.

Regarding fullerene structure, enumeration programs much faster than the standard spiral algorithm, could be developed which allowed, for example, to observe that the number of fullerenes with n vertices is amazingly close to the number of fullerenes with isolated pentagons on $n + 48$ vertices.