

1079-51-390

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Computational Generation of Crystal Nets.

We outline an algorithm that can, in principle, enumerate all crystal nets (up to isomorphism) in geometric realizations of maximal symmetry, and we look at the version of the program currently under development. The program itself consists largely of matrix manipulations, but it relies on geometric group theory as applied to crystallographic point groups. We consider major problems with crystal net enumeration programs (e.g. the fact that isomorphism does not imply isotopy, the problem of optimizing geometric realizations with respect to physical conditions, the problem of the size of the search spaces involved), and describe how they might be addressed in this and subsequent versions. (Received January 18, 2012)