

## Poster Presentation

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### *Crystal Prediction using the Point Groups: an Application of Group Theory*

G. McColm<sup>1</sup>

<sup>1</sup>*University of South Florida, Department of Mathematics & Statistics, Tampa, USA*

As a blueprint for designing a crystal, a crystal net should be a geometric object. So a crystal design regime might be based on an algorithm that generates crystal nets using geometry. The “Crystal Turtlebug” is such a program, generating crystal nets as graphs embedded in 3-space. McColm et al (2011) described a “Maple” version; it generated crystal nets of one or two kinds of vertices and one or two kinds of edges. A new “Python” version can generate crystal nets of any number of kinds of vertices and edges. The algorithm employs matrix representations of point groups. The “core” of the program takes a fragment of the prospective crystal (e.g. for a crystal of 3 kinds of atoms and 2 kinds of bonds, a “transversal” of 3 vertices and 2 edges). The core assigns point groups to the vertices and isometries to the edges. The core then repeatedly applies groups to isometries and vice versa to generate a unit cell. The computational problem is finding a transversal that produces a chemically plausible crystal net, as most crystal nets found are implausible. We follow a breadth-first search and enumerate some transversals, screen them, generate crystal nets from the screened transversals, and screen the results. This process can entail generating millions of transversals to obtain a handful of crystal nets for users to view manually. Although such a geometric approach is somewhat different from the more popular directions of contemporary research in crystal prediction, there is precedent in the work of A. F. Wells, A. Le Bail, C. Wilmer et al, and in particular M. Treacy et al (2004). In principle, the Crystal Turtlebug will generate every crystal net up to topological equivalence. In practice, there is an exponential explosion in the number of transversals, so the time spent enumerating crystal nets within fixed parameters explodes exponentially with the number of kinds of atoms and bonds (McColm (2012)).

[1] G. L. McColm, W. E. Clark, M. Eddaoudi, L. Wojtas, M. Zaworotko (2011), *Crystal Growth & Design* 11:9, 3686., [2] Treacy M. M. J.; Rivin I.; Balkovsky E.; Randall K. H.; Foster M. D. (2004), *Microporous and Mesoporous Materials* 74, 121., [3] G. L. McColm (2012), *J. Graph Algorithms and Applications* 16:2, 507.

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