An algebraic search for large-angle rigid unit modes

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Keywords: rigid unit mode (RUM), irreducible representation, algebraic

Rigid Unit Modes (RUMs), which involve cooperative patterns of polyhedral or molecular rotations and translations, influence a wide variety of important material properties. Recent work provided an algebraic approach to systematically and exhaustively predicting the small-angle RUMs for a given crystal structure, which are classified by irreducible representations of the parent symmetry group of the unrotated structures [1-3]. When some small-angle RUMs are extended to large angles, their rigid units become substantially distorted, indicating that they are not large-angle RUMs. Because large-angle RUMs are also important to many crystalline materials, an algorithm capable of predicting or identifying large-angle RUMs would be very desirable. We report on such an algorithm and its implementation.