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Combinatorial Optimization Algorithms for the Phase Problem in Single-Crystal X-Ray Diffraction.

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The minimal principle model for phase determination has been proposed as a means to find phase invariants that best fit single crystal X-ray diffraction data [1]. This model is a difficult least squares optimization problem with multiple local optima. We develop the first deterministic global optimization algorithms for this model and novel minimal principle models. For the case of centrosymmetric structures, the phases take values of 0 or 180 degrees. This permits the development of a combinatorial optimization formulation for this problem as shown recently in [2]. We reduce this latter problem to the solution of an algebraic system of equations and solve it in polynomial time with a binary Gaussian elimination algorithm. For non-centrosymmetric structures, we proposed a mixed-integer quadratic programming optimization model. Extensive computational results are presented for both models.

References:

- [1] Debaerdemaeker, T. and M. M. Woolfson, On the application of phase relationships to complex structures. XXII. Techniques for random phase refinement, *Acta Crystallographica A*, 39:193-196, 1983.
- [2] Vaia, A. and N. V. Sahinidis, An integer programming approach to the phase problem for centrosymmetric structures, *Acta Crystallographica A*, 59(5), 452-458, 2003.