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**Degree-of-freedom-based Methods for Phasing Centrosymmetric Structures from X-ray Diffraction Data.** A. B. Smith, N.V. Sahinidis, Dept. of Chemical and Biological Engineering, Univ. of Illinois at Urbana-Champaign, Urbana, IL 61801 USA.

The phase problem has recently been approached via combinatorial optimization techniques that are guaranteed to find a global optimum of a certain minimal principle formulation for centrosymmetric structures [1,2]. However, this formulation falls short from accounting for translational symmetry and atomicity constraints.

In this paper, a new integer minimal principle for centrosymmetric structures is presented; one which fully accounts for reciprocal space phase shifts resulting from translational symmetry relations. Additionally, to enforce atomicity constraints, characterization of false minima is done in terms of even and odd triplets. Based on this characterization, an n-best triplet method is proposed: Gaussian elimination using only a subset of reliable triplets. Phase solution sets are generated by enumerating the degrees of freedom present. A reciprocal space solution filter is introduced to further decrease the number of candidate phase solutions. Computational results are presented for a few challenging structures.

References

- [1] A. Vaia and N.V. Sahinidis. An integer programming approach to the phase problem for centrosymmetric structures. *Acta Crystallographica A*, 59:452–458, 2003.
- [2] A. Vaia and N.V. Sahinidis. Polynomial-time algorithms for the integer minimal principle for centrosymmetric structures. *Acta Crystallographica A*, 61:445–4528, 2005.