

## Some Reminiscences of Non-centrosymmetric Structures

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In the “neanderthal” age of crystallography, a light atom non-centrosymmetric crystal was usually relegated to the skeleton collection of unsolvable structures. The development of MULTAN and its increasingly sophisticated successors has made consideration of centrosymmetry essentially a non-issue in structure solution and refinement.

Nevertheless, the question of the relationship between molecular symmetry and crystallographic symmetry remains one of considerable importance, especially with regard to crystal engineering and the interest in engineering non-centrosymmetric crystals, for instance for the generation crystals exhibiting non-linear optical effects.

Kitaigorodskii [1] claimed that centrosymmetric molecules essentially universally crystallize in centrosymmetric space groups. However, many molecules lacking a center of symmetry also tend to crystallize in centrosymmetric space groups, e.g.  $P2_1/c$ ,  $P1\text{-bar}$ ,  $C2/c$ , etc. While chiral molecules must crystallize in chiral space groups, it is not clear why some achiral molecules also do so. In the case of polymorphic systems some members may be centrosymmetric and others non-centrosymmetric, providing clues as to how one might achieve a desired either one of the situations.

This presentation will include a number of examples from our own work, in addition to some possible strategies for the generation of centrosymmetric or non-centrosymmetric structures.

[1] Kitaigorodskii A.I., *Organic Chemical Crystallography*, Consultants Bureau, New York, 1961.

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