Determination of structure of CoS_2 by the means of a simple new method; a solution to the phase problem for centrosymmetric cubic crystals

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The result of atoms and centrosymmetric cubic space groups is that an approximate structure of the crystal is contained or embedded in the many peaks of the calculated electron densities [1]. The number of peaks is finite. In this article, we use a systemic and routine method to identify peaks of this approximate structure for CoS_2. All peaks along the diagonal of the unit cell are located. There are four Co and eight S atoms in a unit cell. The four Co atoms must be in (4*a*) or (4*b*) positions. The eight S atoms must be in (8*c*) positions. We use all sixteen combinations of the peaks, subjected to these constraints. For each combination, we use refinement by the minimization of the *R* factor. Two structures of CoS_2 are determined. About this simple new method, we have some remarks:

(i) The method is a simple deterministic method. Chemical knowledge and environment about each atom is not used. Isomorphic replacements are not employed. Only diffraction intensities are employed. This is purely a method in X-ray crystallography. Non-crystallographers may apply this method or the procedures in [1] to solve simple crystal structures.

(ii) All or most hydrogen atoms, light atoms and heavy atoms are located.

(iii) If we have more than one computer, these computers may be used in parallel for the combinations.

(iv) If there is more than one structure which satisfies the experimental diffraction intensities, all these structures may be determined by this method.

(v) In principle, this method can be applied to determine the structure of a very large protein. Structures of all centrosymmetric cubic crystals can be determined. In practice, we will use the procedures in [1].

(vi) We may regard this method as a solution to the phase problem for centrosymmetric cubic crystals.

(vii) If we try to apply this method to a complicated structure, the number of the combinations will be very large. If we include knowledge of environment about each atom, we can significantly reduce the number of combinations.

(viii) The procedures in [1] and the simple new method in this article represent some basic and new knowledge in X-ray crystallography. Much more work can be done. Crystallographers with expertise in the Patterson function or direct methods may combine these with this simple new method.

(ix) If we can obtain an answer to one of two questions in [1], the peaks in the calculated electron densities may follow the trend of atomic numbers. This greatly reduces the number of combinations.

[1] Yuen, P. S. Result of using atoms and centrosymmetric cubic space groups. (Unpublished).

Keywords: approximate structure; constraints; combinations;