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Systematic Absences Corresponding to False Symmetry

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The presence in a crystal of screw axes or glide planes is accompanied by certain systematic absences in the x-ray reflections. It is recognized that special arrangements of atoms can cause weak reflections which may be mistaken for systematic absences, especially in the cases of screw axes where the number of relevant reflections observed may be quite small.

There exists, furthermore, a kind of special arrangement, of which an unlimited number of examples can be constructed, in which the absences will be indeed systematic but without the corresponding symmetry. Consider the atoms divided into two or more sets. The members of the first set have positions related, for example, by a set of glide planes. The members of the second set have positions related by a set of glide planes parallel with but not coincident with the first set. Similar statements apply to the other atomic sets, if any. None of these "glide planes" are properties of the total assembly, because none operates properly on all the atoms. The structure factor of the crystal is zero for reflections corresponding to absences for such a glide plane, however, and thus the intensity data would suggest the presence of the glide plane. This follows from the fact that for appropriate $hk\ell$ each set has zero structure factor, and the total structure factor is a vector sum of the set structure factors. For the absences to be perfect, of course, the electron density of each set must correspond to the "glide planes," as it will if the atoms are spherical.

Similar examples can be constructed in obvious ways for screw axes, for combinations of screw axes and glide planes, or for combinations of non-primitive translations with screw axes and glide planes. Any extinction rule common to the "symmetries" of the sets will be obeyed by the total assembly.

Consider four pairs of atoms in space group $P2_1$, in positions $x,y,z;\bar{x},1/2+y,\bar{z}$ with x,y,z respectively:

m,n,p

m,t-n,1/2+p

q,r,s

q,u-r,1/2+s

If t and u are unequal (mod 1/2) the correct space group is $P2_1$ and there is no center of symmetry, though the absences would correspond to $P2_1/c$ with a center of symmetry.

This kind of arrangement is rare or perhaps even nonexistent in Nature. But it is not unreasonable that it could occur in order substitution or defect structures with large unit cells which are based on simple substructures. Such statements as "The systematic absences prove that the space group is $P2_1/c$", of which I have been guilty as have others, are to be deplored. It does not seem to be unreasonable to say that the space group is determined only when a structure is found which is in satisfactory agreement with the data. We should remember that probable space group means just that.

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