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UNIVERSITY of PENNSYLVANIA

PHILADELPHIA, PENNSYLVANIA 19104

Department of Chemistry

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Dr. Francis Crick
MRC Laboratory of Molecular Biology
Hills Road, Cambridge CB2 2QH
England

Dear Francis,

It is my understanding that in order for a group of reflections from an acentric structure to be effectively centric that these reflections constitute a zone the axis of which is a two-fold axis in the structure, such as the (h0ℓ)'s in $P2_1$, or the (hk0)'s, (h0ℓ)'s, and (0kℓ)'s in $P2_12_12_1$, or the (hhℓ)'s in $P\bar{4}m2$. It would be easy to see if this were not true for a DNA model if the table of F_{calc} had been published, but unfortunately this is not the case.

Although there are numerous twofold axes in some models of one molecule these are not present in the structure as a whole, a condition necessary for centric projections in certain directions.

But this is really a red herring. I took the stand that my reply should not cover every point in nauseous detail, otherwise no-one would read it. It simply is not true that "in centric structures my arguments have much less force". Numerous errors have been made with centric Fouriers. To show this, however, would have required lengthy documentation which not only would not have been appreciated by the general reader of SCIENCE but would have put him to sleep. Most of this was removed from early drafts of my first paper on the advice of shrewd referees. Such as:

1. p-nitroaniline, Acta Cryst. 9, 960 (1956). This corrects an earlier error in which two incorrect centric projections had led to a structure with absurd intermolecular distances. In the correct structure 21 out of 70 F's changed sign for one of the projections. I haven't made the count for the other one. The two incorrect projections were considered plausible by the authors - and the referees and the editor and numerous others who cited that paper.

2. triphenylene, Acta Cryst. 3, 165 (1950). The centric (hk0) projection, Fig. 2, was later shown to be incorrect in Acta Cryst. 7, 595 (1954); see also Acta Cryst. 9, 173 (1956). 60 out of 105 F's changed sign in the correction. Many atoms moved several Å with respect to each other in the correction.

3. β-selenium, Acta Cryst. 5, 236 (1952). In this determination two centric projections were correct, one was incorrect. In the correction, Acta Cryst. 6, 71 (1953) one atom (of eight) was erased and manufactured elsewhere, and the intermolecular relationships was grossly changed. The number of sign changes is not known becuase the first author did not publish an F_o us F_c table for the projection in question. (I do wish authors would publish F tables.)

4. is[illegible]-leucine, Acta Cryst. 7, 703 (1954). Fig. 2a is correct, Fig. 1 is incorrect. They differ in the relative configurations at C_α and C_β. Out of 120 F's for this centric projection only eight differ in sign, and of these seven were of medium weak intensity and one was of medium intensity!

There are many more examples in my notes, but I think that the above suffice to illustrate that it is easy to go wrong by assuming that a particular model is correct and then "proving" it by calculating an electron density function on that basis, whether or not signs or general phases are required. I saw no point in bringing this up in my reply to your comments, but restricted myself to the dyad question.

Anne Sayre and someone named Flint have embarked on a biography of Rosalind Franklin. I suspect that they'll want your version (if they haven't got it already).

Yours,

Jerry Donohue

JD:pm

P. S. Grandpa came from Cork, so note that I am an -ohue, not an -ahue.