15 JUN 1970

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Department of Chemistry

9 June 1970

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Dear Francis:

I have before me your letter of May 6. Although you may find it amusing to believe that I have not appreciated the point about the dyads in the DNA model, I find it nothing less than scandalous that even when this point is explained to you, you still maintain your original erroneous position. The dyads in the model do not lead to numerous effectively centric reflections, and if you don't believe me ask Struther for the calculated A's and B's - you will find that there are not numerous F's with B = O. Hypersymmetry may affect the distribution of the magnitudes of the F's (the N(z) test) but it will not lead to what you call numerous effectively centric reflections.

However, as I have already pointed out, even if the above were true, my original point is still valid, viz., that presentation of a Fourier based on a model does not provide proof of that model, whether or not the structure is centric or acentric. You now bring up an entirely new point and state that it is far harder to get false structures from polymers than from single crystals of small molecules. I note that you merely assert it is far harder, but not impossible. This is fortunate, because a structure proposed for a rather simple polymer in Physica 23, 746 (1957) and Acta Cryst. 20, 341 (1966) was later shown to be incorrect in J. Chem. Phys. 51, 348 (1969) and Acta Cryst. B25, 2168 (1969). Thus, even if it were true that a polymer imposes greater restrictions on a Patterson these restrictions are not severe enough to prevent arriving at a false solution. However, is it not a fact that these restrictions do not apply to the low resolution DNA data? At 3Å most crystals are polymers.

Of course I can explain Fig. 2 on p. 1701, as well as Fig. 1 which comes from another source. What I cannot explain is figures such as occur in JMB 11, 391 (1965) and elsewhere. Perhaps it is significant that the latter were made using experimental data, whereas 1 and 2 above were made with synthetic error-free F's.

But enough of these red herrings. The question is Does model building followed by electron density calculation furnish proof of a structure?

Have not seen anything further about that horse.

Yours,

Jerry

Jerry Donohue

JD:er