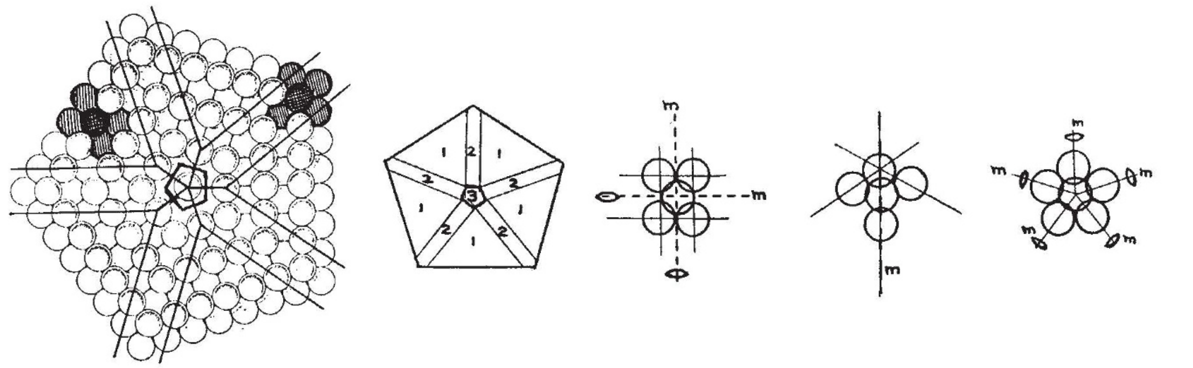
LETTERS TO THE EDITOR

PHYSICS

A Dense Packing of Hard Spheres with Five-fold Symmetry

MR. B. G. BAGLEY's interesting letter[1] on this topic, by making contrasts with quintuple twins, seems continually to argue that his structure should be regarded as one pentasymmetric crystal. I suggest that this notion is invalid on two distinct grounds.

By definition, a crystal is an aggregate of particles such that each identical or 'equivalent' particle has an identical spatial environment, which includes not only co-ordination number—here always 10—but also co-ordination angles and distances. Also, by definition, the symmetry elements of a single, continuous crystal lattice can be found at 'any' place within such a structure. In the assemblage proposed by Bagley: (*a*) all the identical particles (his 'hard spheres') do not have identical spatial environments, and (*b*) the symmetry elements of one 'place' in the assemblage differ from those at other 'places'. His assemblage has, in fact, three distinct types of 'place': (1) a 'general' place; (2) a planar place; (3) an axial place—the last two being normal to the plane of the diagram (Fig. 1). Place (1) has orthorhombic symmetry; place (2) has monoclinic (*m*, 'Domatic'); place (3) pentagonal symmetry.



A B C D E

Fig. 1. *A*, "A layer of hard spheres based on a packing sequence of concentric pentagons." *B*, The three symmetry places. *C*, Orthorhombic unit from place (1). *D*, Monoclinic (*m*) unit from place (2). *E*, Pentagonal unit from place (3)

Because only place (1) is 'general', in being three-dimensional, this seems to show quite unequivocally that the assemblage is, and must be regarded as, a perfect quintuple orthorhombic twin, the five distinct portions joining each other at place (2) and place (3). Even Bagley does not seem fully convinced, as he makes a point of remarking (end of second paragraph) that the assemblage "has a *unique* axis, the *single* 5-fold rotation axis" (my italics).

Any notion that the structure is one crystal because a particular tetrahedron (Bagley's 5·15 per cent distorted one) can be found *throughout* the structure is quite invalid as (*a*) this is also true of any twinned crystal, and (*b*) the conjunctions of identical tetrahedron are different in the three regions of the assemblage. Finally, as in this structure the co-planar 'concentric' pentagons do not touch each other, no known packing mechanism would account for the continual planar growth of these concentric pentagons—a fact strongly supporting the purely five-fold axis propagation direction of extremely 'narrow' quintuple-twin 'whiskers', from some initial (and fortuitous ?) five-sphered planar ring.

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[1] Bagley, B. G., *Nature*, **208**, 674 (1965).

PROF. J. D. BERNAL * writes:

"I agree with Mr. Clarke's criticism of Mr. Bagley's communication. The arrangement he illustrates is definitely a twin in terms of classical crystallography for the reasons which he gives. However, this seems to me more a matter of amending precise definitions of the laws of crystallography than of insisting on them. If precise equality of interatomic distances is not required, arrangements forbidden by these laws can occur. They do, in fact, occur, not only in the cases mentioned by Mr. Bagley but also in structures of many polyhedral viruses, as discussed by Dr. A. Klug and Dr. D. L. D. Caspar[1]. Furthermore, the arrangement Mr. Bagley shows is quite a special one of pentagonal symmetry in a plane. Far more general is the arrangement in an icosahedral shell which has been described by Dr. A. L. Mackay (see Fig. 7, ref. 2). This possesses not a single five-fold axis but six of them. In other words, it has symmetry 532 but is nevertheless strictly a polysynthetic twin with orthorhombic elements. The origin of twins is not, in my opinion, at all difficult to explain. Ideally, a crystal lattice consists of an infinite number of particles all similarly situated. When the number is finite, it is impossible to satisfy the condition for each particle. It can never be similarly surrounded by others. Surface effects are bound to influence the arrangement of the particles when they are only of the order of a few hundreds of them. I have discussed the existence of such nuclei which I have referred to as pseudonuclei[3] which can never grow extensively and all crystallographers will have noticed that precipitated nuclei are often twinned from the start."

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[1] Klug, A., and Caspar, D. L. D., *Cold Spr. Harb. Symp. Quant. Biol.*, **27**, 1 (1962).
[2] Mackay, A. L., *Acta Cryst.*, **15**, 916 (1962).
[3] Bernal, J. D., *Proc. Roy. Soc.*, A, **280**, 299 (1964).