

Crystal Structure of Diamond

IN a recent communication in *Nature*¹, Mrs. Lonsdale has questioned the statement made by Sir C. V. Raman² that the X-ray data leave the question whether diamond possesses tetrahedral or octahedral symmetry of structure entirely open. The present communication is a reply to some of the specific points raised in her letter.

As is well known, the structure of diamond consists of two interpenetrating face-centred cubic lattices, the two atoms in the basis having the co-ordinates 000 and $\frac{1}{4}\frac{1}{4}\frac{1}{4}$. From the fact that the atoms occupy these special positions in the lattice, it follows that they must possess tetrahedral (*Td*) symmetry of structure, which may be visualized by drawing a set of planes passing through the atomic nucleus and parallel to the cubic and dodecahedral planes, and thereby dividing up the whole electronic cloud into 48 pyramids. Tetrahedral symmetry requires that if the charge distribution in one of these pyramids is specified, those in 23 others should also be the same, these 24 pyramids being distributed (six each) in four non-adjacent octants of the sphere drawn round the nucleus. The charge distributions in the remaining 24 pyramids would also be identical, but different from those in the first set.

As a consequence of the tetrahedral symmetry of the atoms, the crystal as a whole would also possess the same symmetry, except in the special case when the electronic states and configurations of the two atoms are exactly identical and geometrically symmetric about a point midway between them ($\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$). It is easily proved, however, that this special relationship, which results in a higher or octahedral symmetry for the crystal, is not a necessary condition either for the non-appearance of the 200 X-ray reflexion nor for the appearance with a low intensity of the 222 X-ray reflexion. The vanishing of the 200 reflexion is secured if the radial distribution of electronic charge, when *summed up* for a pair of

opposed pyramids in each atom, is the same for both the atoms in the basis. This means that the total charge in a spherical shell surrounding the nucleus, and consequently also the integrated total charge, is the same for both atoms. The fact that diamond does not exhibit either piezo- or pyroelectricity thereby becomes intelligible. Further, the 222 X-ray reflexion would only vanish in two special cases, namely, (a) when each atom is octahedrally symmetrical, or (b) when the atoms are tetrahedrally symmetrical, but the radial distributions of charge are identical in similarly directed pyramids in the two atoms.

Prima facie, neither of these special conditions can be expected to exist; as a result of the valence binding, the electronic distribution would in general tend more towards identity in opposing pyramids than in parallel ones. The appearance of a 222 reflexion is thus naturally to be expected. But any departure, however small, from identity and symmetry of the distributions in opposing pyramids would result in the structure as a whole possessing only tetrahedral and not octahedral symmetry. The spectroscopic behaviour of diamond shows beyond all possibility of doubt that this is so in the majority of cases.

G. N. RAMACHANDRAN.

Department of Physics,
Indian Institute of Science,
Bangalore.
May 17.

¹ Lonsdale, K., *Nature*, 155, 144 (1945).

² Raman, Sir C. V., *Proc. Ind. Acad. Sci.*, A, 19, 189 (1944).