Letters to the Editor

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Structure of the Azide Group

IN the account in NATURE of May 26, p. 802, of the recent discussion on dipole moments held at Oxford by the Faraday Society, reference is made to the probable linearity of the arrangement of the nitrogen atoms in the azide group. An X-ray examination of cyanuric triazide made by Miss Knaggs in the Davy Faraday Laboratory shows that this hypothesis is correct. I gave a short account of her work in a lecture at the Royal Institution at the end of last year. The arrangement bears a curious resemblance to the arms of the Isle of Man, a row of three nitrogen atoms lying in the position of each leg from knee to ankle.

FIG. 1. Crystal cell of cyanuric triazide. $AB=CD=8.73$ Å. Broken lines represent molecules separated from that represented by continuous lines by 2.98 Å, parallel to the hexagonal axis of the cell.

Miss Knaggs has now nearly completed a Fourier analysis of the electron distribution in the molecule, which confirms her preliminary determination of the structure. It is a 'layer structure' and resembles that of graphite, but the arrangement in the layers is very different. The molecules are distinct and planar. The layers are closer together than in graphite, being only 2.98 Å. apart as against 3.41 Å. in graphite. The structure is interesting because it furnishes the data of distances between nitrogen atoms, and between nitrogen and carbon atoms, both in the same molecule and in neighbouring molecules.

Cyanuric triazide is highly explosive, which fact may be connected with its high density, 1.71 , which is unusually high for an organic compound.

Fig. 1 shows the size of the cell, which is hexagonal, and the arrangement of the molecules belonging to it. The completed Fourier analysis will give the exact positions of the atoms.

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Orientation of Molecules in the *p*-Benzoquinone Crystal by X-Ray Analysis

K. S. KRISHNAN and S. Banerjee¹ have recently deduced the orientation of the molecular planes in this crystal by a study of the magnetic susceptibilities. The structure is an interesting one because they find that the plane of the benzene ring is almost coincident with the (201) plane of the crystal.

Cases of this kind in which all the atoms of an organic compound are coincident or nearly coincident with a simple crystallographic plane are unfortunately very rare, so it is worth while to inquire to what extent this relationship is an exact one. The magnetic results indicate that the plane of the molecule is inclined about 3° from the (201) towards the *c* axis.

A quantitative X-ray investigation of this structure has now been carried out, and the results are in agreement with the magnetic measurements, but go further, in that the complete orientation of the molecules can be determined, as well as the inclination of their planes. The results show that the small departure of the molecular planes from coincidence with the (201) is quite definite, and also that they are inclined in such a way that the planes of adjacent molecules are not quite parallel. Thus the measured values of *F* for the first three orders of the (201) reflection are 51, 24, and 5.5, as compared with calculated maxima of about 60, 29, and 14, which would apply if all the atoms were in phase. The large falling off in the case of the third order can best be explained by some departure of the atoms from exact coincidence with this plane. Further, any structure placing the atoms strictly in the (201) plane would give the orders of the (200) reflection the same geometrical structure factors as the orders of the (001), whereas there are actually considerable differences.

The crystal is monoclinic, $a=7.03$, $b=6.79$, $c=5.77$ Å., $\beta=101.0^\circ$, space group $P2_1/a$, with two centrosymmetric molecules per unit cell. Assuming a planar model with the oxygen atoms at 1.2 Å. from the benzene carbon, the following orientation is found to give a reasonable quantitative explanation of the intensities of more than seventy reflections which have been measured. The line joining the two oxygen atoms in the molecule makes 79° with the *a* axis of the crystal, 37.5° with the *b* axis, and 54.5° with the normal to the (001). The line at right angles to this, also in the plane of the molecule, makes 70° , 127° , and 44° with these crystal directions. As the dimensions and scattering power of the two oxygen atoms in the molecule are somewhat uncertain, it would be unsafe to estimate the possible error in these figures at less than 3° or 4° at present. But it seems quite certain that the molecular planes depart from parallelism with the (201) by between 3° and 7° .

Starting from the above approximation, the experimental measurements are now being subjected to a Fourier analysis by which it is hoped to obtain more precise information regarding the structure of the molecule.

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¹ NATURE, 131, 653, May 6, 1933.