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An unusual double reflection in α -phenazine. By F. L. HIRSHFELD, Weizmann Institute of Science, Rehovoth, Israel

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During the investigation of the crystal structure of a-phenazine (Herbstein & Schmidt, 1955a, b), an extra spot was observed, corresponding in position to the forbidden 500 reflection, on all hol, but not hk0, Weissenberg photographs, with both Cu and Mo $K\alpha$ radiation, and both at room temperature and in boiling nitrogen. This spot, whose shape and intensity varied for different crystals and even on different photographs of the same crystal, remained unexplained until it was realized that in normal-beam photography about [010] the reciprocallattice points 210 and 310, as well as 210 and 310, cut the sphere of reflection almost simultaneously with 500, this coincidence resulting from the axial ratio $b^*/a^*=6^{\frac{1}{2}}$ and being virtually independent of wavelength. Since 210 and 310 are, respectively, the fourth and second strongest reflections recorded, with observed structure factors of 40.1 and 46.0 at room temperature, the conditions are highly favorable for the appearance of a sizable double reflection in the 500 position. What is particularly unusual in this situation is the fivefold coincidence that permits four distinct kinds of double reflection to arise at the same time, these being $(210+3\overline{1}0)$, $(2\overline{1}0+310)$, $(310+2\overline{1}0)$, and $(3\overline{1}0+210)$.

It might be expected that since, in space group $P2_1/a$, the 210 and $2\overline{10}$ structure factors have opposite signs while 310 and $3\overline{10}$ have the same sign, rays reflected from 210 and $3\overline{10}$, in whichever sequence these reflections occur, should be opposite in phase to those reflected from 210 and 310, with consequent destructive interference between the two pairs of twice-reflected beams. That such destructive interference, if it occurs at all, is far from complete seems to confirm the conclusion of Lipscomb (1949) that interference effects of this sort would ordinarily be unobservable because of the convergence of the X-ray beam and the mosaic character of the crystal. Indeed, the occurrence of the 500 spot in α -phenazine is even more conclusive in this regard than is the failure of such experiments as those of Fankuchen and of Lipscomb to use the interference between single and double reflections for determining phase relationships among the structure factors. For in such experiments, even if the crystal were perfect, the conditions for single reflection would be satisfied, for a given crystal orientation, by a wide range of directions of the incident radiation, whereas only a minute fraction of the incident beam would arrive in precisely the proper direction for double reflection. Under these conditions the effects of interference would probably be imperceptible. In the phenomenon described here, on the other hand, if the crystal were perfect then the same portion of the incident beam would produce simultaneously two coherent double reflections opposite in phase, and interference between them would be complete. For if, at a particular instant, the points 500 and 210 lie on the sphere of reflection corresponding to a particular ray of incident radiation, then the point 310 must simultaneously lie on the same sphere of reflection, this being a necessary consequence of the orthogonality of the a^* and b^* axes. Thus whenever the crystal is so oriented as to produce the double reflection $(210+3\overline{1}0)$, it must simultaneously produce $(310+2\overline{1}0)$ with equal amplitude and opposite phase. The appearance of 500 must, therefore, be due to the mosaic spread of the crystal, which permits, for example, the 210 reflection from one crystal block to be subsequently reflected by the $3\overline{10}$ planes of a second crystal block even though no double reflection is possible in either of these individual blocks. If a similar experiment could be set up with a nearly perfect crystal some degree of destructive interference might be detectable. Such an experiment could be of value in testing the feasibility of interference methods in general for the determination of the relative phases of structure factors.

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