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Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible. Publication will be quicker if the contributions are without illustrations.*

Pseudo-orthorhombic diffraction patterns and OD structures. By K. DORNBERGER-SCHIFF, *Institut für Strukturforschung der Deutschen Akademie der Wissenschaften zu Berlin, Germany,* and J. D. DUNITZ, *Organic Chemistry Laboratory, Swiss Federal Institute of Technology, Zürich, Switzerland*

In a recent publication (Dunitz, 1964) the interpretation of certain pseudo-orthorhombic diffraction patterns was discussed in terms of the twinning of monoclinic structures. We wish to point out here that all the pseudo-orthorhombic patterns discussed in the previous paper can equally well, and perhaps more convincingly, be interpreted in terms of OD (order–disorder) structures (Dornberger-Schiff, 1956, 1964; Dornberger-Schiff & Grell-Niemann, 1961), *i.e.* structures consisting of layers such that pairs of successive layers can be formed in two or more geometrically, and hence energetically, equivalent ways. In some cases the previous conclusions are little altered, except that the twinning is to be understood as OD twinning, but for the cycloundecylamine hydrobromide and cobalt dipyridine dichloride cases the previous interpretations may have to be more radically revised.

Para-orthorhombic structures (monoclinic structures in which the projections down three mutually perpendicular directions have perfect rectangular symmetry) are seen to arise naturally from certain types of OD arrangements. This is illustrated by the example, one of many possible, shown in Fig. 1 left. The example shows an ordered arrangement of layers [symmetry P(2)*mb*] in which the relationship between any pair of successive layers is identical and can be described in terms of a displacement by the stacking vector $s_1 = a_0 + b/4$. This ordered arrangement is para-orthorhombic, space group *P*11*b* (No. 7, C_s^2); because all triples and higher *n*-tuples of successive layers are geometrically

equivalent, such an arrangement is described as having 'maximum degree of order'. We shall refer to it as the arrangement MDO$_1$. Displacement of any layer by *b*/2, corresponding to the occurrence of a stacking vector $s_2 = a_0 - b/4$, gives an interlayer relationship that is geometrically, and hence energetically, equivalent to that in the ordered arrangement. An arrangement containing long sequences of stacking vectors s_1 alternating with long sequences of vectors s_2 would be an OD twin. For shorter sequences we would speak of polysynthetic twinning or – if the ordered
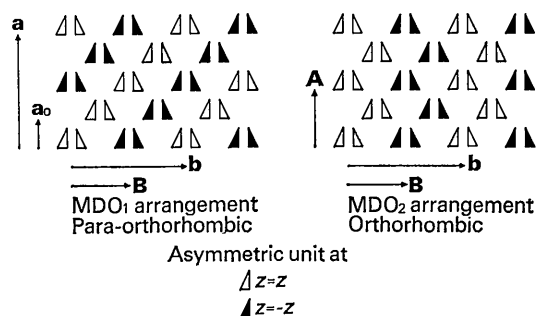

Fig. 1. Schematic representation of two ordered OD-arrangements, MDO$_1$ and MDO$_2$, based on the same layers and pairs of layers; a, b, c non-primitive (fourfold) rectangular unit cell of MDO$_1$ A, B, c unit cell of superposition structure c perpendicular to plane of paper.

regions are small enough to give diffuse streaks parallel to a^* on the X-ray diagrams – of a disordered structure with a predominance of regions of the type MDO_1.

Another fully ordered arrangement (MDO_2) of the same kind of layers and pairs of layers (but different kinds of triples) is shown in Fig. 1 right. Here the stacking vectors s_1 and s_2 alternate regularly to produce an orthorhombic structure, space group $P2_1ab$ (No. 29, C_{2v}^5). An occasional mistake in such a sequence would not result in twinning but in a parallel overgrowth of two orthorhombic crystals shifted $b/2$ with respect to each other. The X-ray diagram would differ from that of the fully ordered structure by a general reduction of the intensities of reflexions with k odd by a factor varying from sample to sample. Again, if the ordered regions are small enough to give diffuse streaks on the X-ray diagrams we can speak of a disordered structure with a predominance of ordered regions of type MDO_2. We could also have ordered regions of both types, MDO_1 and MDO_2; and finally, an arrangement in which the stacking vectors s_1 and s_2 occurred at random with equal probability would correspond to the limit of OD disorder.

In Table 1 the conditions for the occurrence of reflexions and for the symmetry of their intensities are listed for arrangements enumerated from left to right with increasing frequency of changes in the stacking vector. All these arrangements belong to the same 'family of OD structures'; they differ only in the geometrical relationship and inter-action energy between non-adjacent layers, complete disorder implying a vanishing energy dependence between layers separated by $2a_0$.

The 'superposition structure' derived by superimposing any given arrangement with itself shifted by $b/2$ is the same for all members of the family; it is orthorhombic, space group $C2mm$ (No. 38, C_{2v}^{14}) with periodicities $2a_0$, $b/2$, c. This means that the pattern of reflexions with k even has orthorhombic symmetry and is the same, with respect to relative intensities and systematic absences, for all the arrangements (see Table 1).

Features of the kind summarized in Table 1, or rather a selection of them, are shown by most of the para-orthorhombic structures that have been examined. A more detailed reinterpretation of pseudo-orthorhombic diffraction patterns in terms of OD arrangement is now being prepared (Dornberger-Schiff, to be published).

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Table 1. *Conditions limiting possible reflexions and symmetry of intensities*

| | Ordered MDO_1 | Twin MDO_1 | Disordered | | | | Parallel intergrowth MDO_2 | Ordered MDO_2 |
| | | | Ordered regions | | Complete disorder | Ordered regions | | |
			MDO_1	MDO_1 and MDO_2				
Translation a	$a_0 + b/4$							$2a_0$
Space group	$P\,1\,1\,b$							$P2_1ab$
(ξkl) with* $k = 2n+1$	$h+k=4n$	$h+k=2n$	Maxima for $\xi+k=2n$ / $\xi=h$			Maxima for $\xi=2H$	$h=2H$	
	$I(hkl)=I(hk\bar{l})$ $I(hkl)\neq I(\bar{h}kl)$	$I(hkl)=I(hk\bar{l})$ $I(hkl)=I(\bar{h}kl)$ (possibly)				$I(hkl)=I(hk\bar{l})=I(\bar{h}kl)$		
$(\xi k0)$ with* $k = 2n+1$	Reflexions missing							
(ξkl) with* $k = 2K$	$\xi=2H$ $H+K=2n$ $I(hkl)=I(hk\bar{l})=I(\bar{h}kl)$							

* Referred to unit cell $4a_0$ b c; ξ continuous; h, H, K, n integral values.