to the order (n) of the characteristic Bessel functions is not readily answered from a study of (33) and (34). We consider that (33) and (34) are correct: the order number n does not appear explicitly in these equations, however.

Computer simulation of $I_{pd}(\xi, l)$ in Figs. 4(a) and (b) show that axial disorder has little influence on layer line $l=7$, $n=1$, whereas it has a noticeable effect on layer line $l=1$, $n=2$. The case of $l=0$, $n=0$ (which is not shown) resembles the case of $l=7$, $n=1$ in that the $l=0$ profile is little changed by axial disorder. Thus, the diffracted intensity $I_{pd}(\xi, l)$ as defined by (33) and (34) tends to show that axial disorder is directly related to the order (n) of the characteristic Bessel functions. It might be thought that the M and N values play an important role as they define the value of the radius Δ_m. Recall that $D_m(\xi)$ values are insensitive to axial disorder when Δ_m approaches $2r_0$. However, the calculated $I_{pd}(\xi, 3)$ and $I_{pd}(\xi, 6)$ profiles for the collagen helix with parameters of $M=10$, $N=3$ and with the same amount of axial disorder are identical to those in Figs. 4(a) and (b) respectively, after allowing for the different r_0 parameters. Thus, the n dependence of axial disorder is inherent in the framework of (33) and (34).

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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.*

Acta Cryst. (1989). A**45**, 654-656

Experimental phase effects and X-ray wavelengths. By BEN POST, JOHN DIMARCO and WALTER KISZENICK, *Physics Department, Polytechnic University, Brooklyn,* 11201 *New York, USA*

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Abstract

It is shown that Shen & Colella [*Acta Cryst.* (1986). **A42**, 533-538; *Nature (London).* (1987). **329**, 232-233; *Acta Cryst.* (1988). **A44**, 17-21] are in error in asserting that 'irrespective of instrumental resolution' asymmetric n-beam benzil interactions can be recorded only if incident-beam wavelengths equal to, or greater than, 3·5 Å are used. Such interactions are clearly displayed in our Cu $K\alpha_1$ and Cr $K\alpha_1$ n-beam patterns of organic crystals, such as benzil, and that useful phase information can be readily extracted from such data.

In recent publications, Shen & Colella (1986, 1987, 1988), referred to below as 'S&C', described difficulties they encountered in their efforts to record asymmetric interaction maxima in n-beam patterns of organic acentric benzil crystals. In discussing results obtained with Cu $K\alpha_1$ and Cr $K\alpha_1$ they state that 'so far we have not been able to see the asymmetric effects in the wings of the Renninger peaks.' Their negative results were attributed to the very small half-widths and asymmetries of the benzil maxima, and to inadequacies of the instrumentation then available to them, *i.e.* 'the resolution needed on the φ scale ($\simeq 1'$) is not normally available in standard laboratory experiments. The only way to achieve this kind of resolution is to use a beam from a synchrotron light source' (Shen & Colella, 1986, p. 537).

We are aware of the many advantages of synchrotron X-ray sources over conventional ones. Clearly, they can

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provide incident beams with small divergence, but, equally clearly, they do not represent 'the only way to achieve this kind of resolution'.

More recently, S&C wrote that 'initially we were not able to see any VBS* effect, even when a highly collimated beam from a synchrotron source was used.... It became clear that, irrespective of the instrumental resolution, no VBS effects could be observed in a crystal like benzil.... Further calculations showed that at a wavelength of 3·5 Å pronounced asymmetry effects were visible in the azimuthal plots of the 202 reflection...' (Shen & Colella, 1987).

We are unable to reconcile the S&C statements cited above with the results of our investigations of n-beam patterns of benzil. Benzil is a trigonal crystal with $a = 8{\cdot}409$ and $c = 13{\cdot}672$ Å; the setting corresponds to space group $P3_121$. At a meeting of the American Crystallographic Association, at the University of Texas in the Spring of 1987, one of us presented a paper which included displays of several asymmetric [006] n-beam interactions recorded with Cu $K\alpha_1$ radiation (Post, 1987). Examples are shown in Fig. 1. These were obtained by reflection from and transmission through a 2 mm thick 'needle' grown by evaporation from solution in an organic solvent.

We have also recorded twenty asymmetric n-beam benzil interactions in the 90° asymmetric portion of a [030] scan using Cr $K\alpha_1$ radiation. A Rigaku Denki rotating-anode generator, run at a total power input of 1·6–2·0 kW, provided the incident radiation. The actual target size, $0{\cdot}3 \times 3$ mm was reduced to an effective size of $0{\cdot}3 \times 0{\cdot}2$ mm by using a take-off angle of 4°. The incident beam divergence was reduced to about 45″ arc by moving the center of the crystal goniometer to a position 2·2 m from the target. The goniometer was separated from the target by an evacuated pipe fitted with thin Mylar windows at both ends. The incident beam emerged from the pipe *via* a 0·5 mm pinhole close to the crystal.

Some of the interactions are shown in Figs. 2, 3, and 4; relevant data are listed in Table 1. The azimuthal angles at which interactions were detected are listed under 'θ'; under the heading 'I/O' (*i.e.* 'in' or 'out'), we indicate whether

* The term VBS ('virtual Bragg scattering') is used by S&C to describe cases in which the primary reflection is 'weak but strongly excited, while the simultaneous reflection is strong but weakly excited' (Shen & Colella, 1987).

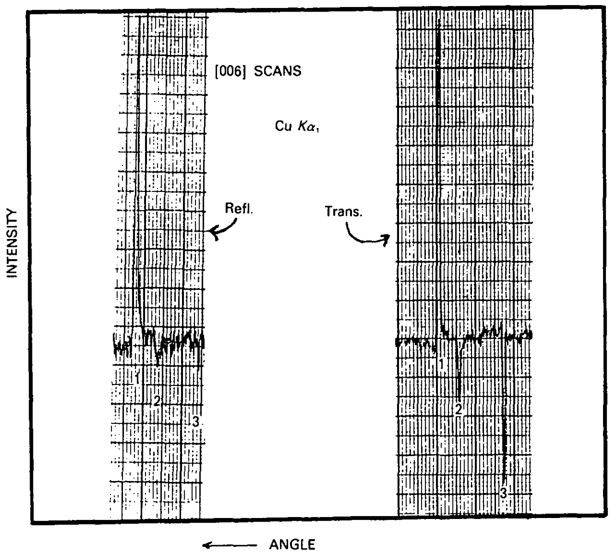

Fig. 1. Small portion of [006] n-beam pattern, recorded in reflection and transmission. Cu $K\alpha_1$.

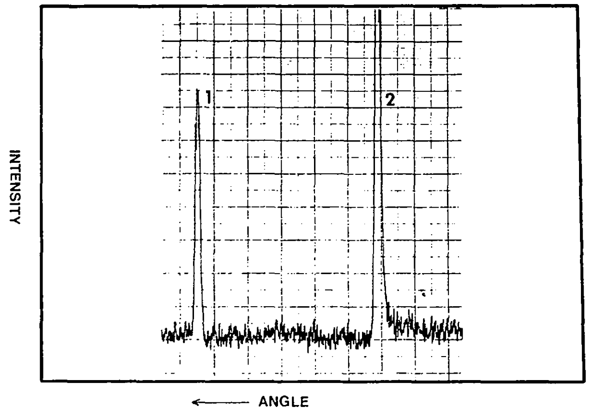

Fig. 2. Two four-beam [030] interactions. Cr $K\alpha_1$.

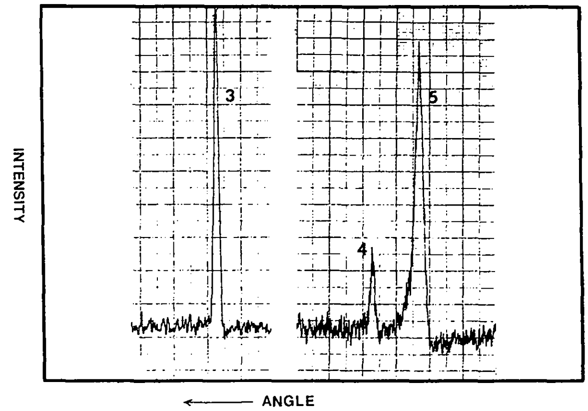

Fig. 3. Three-, four- and six-beam interactions. Cr $K\alpha_1$.

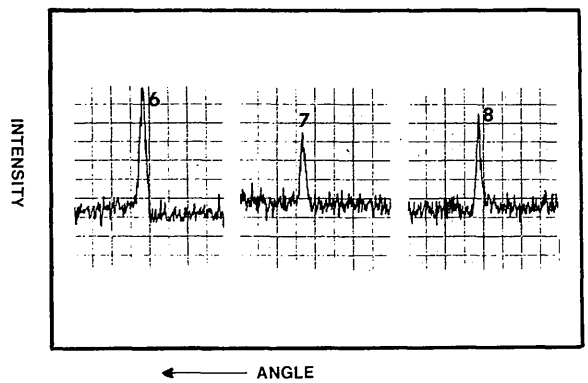

Fig. 4. Asymmetries displayed by weak interactions. Cr $K\alpha_1$.

Table 1. *N-beam interactions*; [030] *benzil*; Cr $K\alpha_1$

Peak no.	θ	Number of beams	Experimental I/O	Experimental R/L	Experimental Sign	Indices r.l.p.	Indices coupling
1	55·62	4	I	R	+	$\bar{1}1\bar{2}$	122
						$\bar{1}3\bar{2}$	102
2	54·94	4	I	L	−	$02\bar{1}$	011
						$01\bar{1}$	021
3	43·91	3	O	R	−	111	$\bar{1}2\bar{1}$
4	30·97	6	I	R	+	(indices omitted)	
5	30·76	4	O	R	−	$0\bar{1}2$	$04\bar{2}$
						042	$0\bar{1}\bar{2}$
6	79·05	4	I	R	+	$\bar{1}4\bar{2}$	$1\bar{1}2$
						$\bar{1}0\bar{2}$	$1\bar{3}2$
7	53·61	3	O	R	−	112	$\bar{1}2\bar{2}$
8	35·94	4	I	L	−	$\bar{2}1\bar{1}$	221
						$\bar{2}4\bar{1}$	$2\bar{1}1$

the corresponding reciprocal-lattice point (r.l.p.) is entering or leaving the Ewald sphere; under 'R/L' we indicate the location of the intensity minimum, to the right or left of the interaction maximum; the experimentally determined sign of the invariant phase is given in the adjacent column. The indices of the r.l.p.s and their coupling terms are given in the last column.

It is clear that abundant useful n-beam data for benzil and similar crystals can be recorded with Cu $K\alpha_1$, Cr $K\alpha_1$ and other radiations. [A detailed study of experimental determinations of the signs of invariant benzil phases has been prepared by one of the authors (BP) for submission to *Acta Cryst.* Section A.] It should also be clear that failure to observe an experimental effect may be due to factors other than the total absence of the effect.

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Acta Cryst. (1989). A**45**, 656

On integrating the techniques of direct methods with anomalous dispersion: the one-phase structure seminvariants in the monoclinic and orthorhombic systems. III. Primitive non-centrosymmetric space groups of type 1*P*220.

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Abstract

In a recent paper by Velmurugan & Hauptman [*Acta Cryst.* (1989), A**45**, 158-163], conditional probability distributions were derived for the one-phase structure seminvariants in the presence of anomalous scattering for the monoclinic system and for the space groups of type 1*P*222 in the orthorhombic system. This paper is an extension of the above paper for the primitive non-centrosymmetric space groups of type 1*P*220 in the orthorhombic system. The one-phase structure seminvariants are of the form $\Phi_{2h'2k'0}$. Since the theory for this case was treated in the earlier paper, only a brief summary of results is given here.

Summary of final results

Ten space groups (Table 1) fall in the category 1*P*220. For the derivation of the conditional probability distributions for the one-phase structure seminvariants $\Phi_{2h'k'0}$ in this category the reader is referred to Velmurugan & Hauptman (1989), in particular § 5.2 and column 2 of Table 1. The relevant P values for the ten space groups are listed in Table 1 below. With equations (9.3) of the earlier paper and the new P values for these ten space groups, the corresponding conditional probability distributions can be obtained from equation (9.1).

Table 1. *P values for the ten space groups of type* 1*P*220

Space group	P
$Pmm2$	1
$Pmc2_1$	$(-1)^l$
$Pcc2$	1
$Pma2$	1
$Pca2_1$	$(-1)^l$
$Pnc2$	1
$Pmn2_1$	$(-1)^{l+h}$
$Pba2$	1
$Pna2_1$	$(-1)^l$
$Pnn2$	1

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Velmurugan, D. & Hauptman, H. A. (1989). *Acta Cryst.* **A45**, 158-163.

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