Table 11. *Cumulative statistics of the triplet phase sums for different doublet estimations: structural type* 1

SIRNAS case (true sign for the doublets); structure $Pt-C_{744}N_{191}O_{264}$; space group $P1$; resolution 2.3 Å; radiation Cr $K\alpha$; strongest 250 $|E_H|$ values used; DR=0.29.

JPD				PAT			
W	NTR	AER	ERR	*W*	NTR	AER	ERR
1.0	103	88	88	2.0	135	66	70
0.5	413	126	126	1.0	520	71	80
0.0	860	169	169	0.0	864	88	104

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SHORT COMMUNICATIONS

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The asymmetric unit of X-ray intensity data of the seven crystal systems.

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Abstract

A crystal structure can be determined from the X-ray intensity data of one asymmetric unit. As the function $I(hkl)$ of the X-ray intensity has a center of symmetry if it is assumed that anomalous scattering is negligible, $I(hkl)$ has the symmetry of a centrosymmetric point group, *i.e.* a Laue group. The asymmetric units of the intensity data are derived here for all Laue groups.

1. Introduction

The Laue group, together with a corresponding asymmetric unit of X-ray intensity data, must be known to determine a crystal structure. The asymmetric units of intensity data reported so far are incomplete and even contain errors (Sakurai, 1986; Stout & Jensen, 1989). In the present paper, an explanation of how to derive the equivalent intensities for each of the 11 Laue groups is given. The exact extents of the 11 asymmetric units of intensity data are shown.

2. Theory

There is only one Laue group in each of the triclinic, monoclinic and orthorhombic systems but two Laue groups in each of the tetragonal, trigonal, hexagonal and cubic systems. Thus there are 11 Laue groups altogether.

In the trigonal system there exist two Laue groups, $\bar{3}$ and $\bar{3}m$. Both are compatible with a rhombohedral lattice as well as with a hexagonal lattice. Therefore, in Table 1, the point groups $\bar{3}$ and $\bar{3}m$ are described with rhombohedral

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Table 1. *The asymmetric units of intensity data for the* 11 *Laue groups*

Crystal system	Non-centrosymmetric point groups	Laue groups	Asymmetric unit	Fraction of reciprocal space
Triclinic	1	$\bar{1}$	$0 \le h < \infty$, $-\infty < k, l < \infty$ Exclude either $0kl$ if $k < 0$ and $00l$ if $l < 0$ or $0kl$ if $l < 0$ and $0k0$ if $k < 0$.	1/2
			$0 \le k < \infty$, $-\infty < h, l < \infty$ Exclude either $h0l$ if $l < 0$ and $h00$ if $h < 0$ or $h0l$ if $h < 0$ and $00l$ if $l < 0$.	
			$0 \le l < \infty$, $-\infty < h, k < \infty$ Exclude either $hk0$ if $h < 0$ and $0k0$ if $k < 0$ or $hk0$ if $k < 0$ and $h00$ if $h < 0$.	
Monoclinic	2, m	$2/m$ (b axis unique)	$-\infty < h < \infty$, $0 \le k, l < \infty$ Exclude $hk0$ if $h < 0$.	1/4
			$-\infty < l < \infty$, $0 \le h, k < \infty$ Exclude $0kl$ if $l < 0$.	
		(c axis unique)	$-\infty < h < \infty$, $0 \le k, l < \infty$ Exclude $h0l$ if $h < 0$.	
			$-\infty < k < \infty$, $0 \le h, l < \infty$ Exclude $0kl$ if $k < 0$.	
Orthorhombic	222, $mm2$	mmm	$0 \le h, k, l < \infty$.	1/8
Tetragonal	4, $\bar{4}$	$4/m$	$0 \le h, k, l < \infty$ Exclude either $0kl$ if $k > 0$ or $h0l$ if $h > 0$.	1/8
	422, $4mm$	$4/mmm$	$0 \le h \le k < \infty$, $0 \le l < \infty$.	1/16
	$\bar{4}2m$		$0 \le k \le h < \infty$, $0 \le l < \infty$.	
Trigonal	3	$\bar{3}(R)$	$0 \le k, l < \infty$, $-\infty < h \le k, l$ Exclude either hkh if $h < k$ or hhl if $h < l$ and either $h0l$ or $hk0$ if $h < 0$.	1/6
			$0 \le h, l < \infty$, $-\infty < k \le h, l$ Exclude either hkk if $k < h$ or hhl if $h < l$ and either $hk0$ or $0kl$ if $k < 0$.	
			$0 \le h, k < \infty$, $-\infty < l \le h, k$ Exclude either hkh if $h < k$ or hkk if $k < h$ and either $0kl$ or $h0l$ if $l < 0$.	
		$\bar{3}(H)$	$0 \le h, k < \infty$, $-\infty < l < \infty$ Exclude $h0l$ if $l < 0$ and $0kl$ if $l \le 0$.	
	32, $3m$	$\bar{3}$m(R)	$0 \le k \le l < \infty$, $-\infty < h \le k < \infty$ Exclude $h0l$ if $h < 0$ and $\lvert h \rvert > 1$.	1/12
			$0 \le l \le h < \infty$, $-\infty < k \le l < \infty$ Exclude $hk0$ if $k < 0$ and $\lvert k \rvert > h$.	
			$0 \le h \le k < \infty$, $-\infty < l \le h < \infty$ Exclude $0kl$ if $l < 0$ and $\lvert l \rvert > k$.	
		$\bar{3}1m(H)$	$0 \le h \le k < \infty$, $-\infty < l < \infty$ Exclude $0kl$ if $l < 0$.	
			$0 \le k \le h < \infty$, $-\infty < l < \infty$ Exclude $h0l$ if $l < 0$.	
		$\bar{3}m1(H)$	$0 \le h, k, l < \infty$ Exclude either $hk0$ if $h < k$ or $hk0$ if $h > k$.	
Hexagonal	6, $\bar{6}$	$6/m$	$0 \le h, k, l < \infty$ Exclude either $0kl$ if $k > 0$ or $h0l$ if $h > 0$.	1/12
	622, $6mm$	$6/mmm$	$0 \le h \le k < \infty$ $0 \le l < \infty$.	1/24
	$\bar{6}2m$		$0 \le k \le h < \infty$ $0 \le l < \infty$.	
Cubic	23	$m\bar{3}$	$0 \le h \le k, l < \infty$ Exclude hkh if $h < k$.	1/24
	432, $\bar{4}3m$	$m\bar{3}m$	$0 \le h \le k \le l < \infty$.	1/48

R: Rhombohedral coordinate axes.
H: Hexagonal coordinate axes.

and hexagonal lattices. Furthermore, the point group $\bar{3}m$ in the hexagonal description is further subdivided into two cases - one having the normal of the mirror planes in the [100] direction and the other one having the normal in the [210] direction. The Laue group $2/m$ is also subdivided into two cases - with the b axis unique and with the c axis unique.

Since the distribution of the X-ray intensity $I(hkl)$ in reciprocal space shows the same symmetry as a general crystal form of the corresponding Laue class, the asymmetric unit of X-ray intensity data for a crystal is the same as that for the crystal forms $\{hkl\}$ with the symmetry of its Laue group.

Table 1 shows information on the 11 Laue groups (column 3). The crystal system is given in column 1, all corresponding noncentrosymmetric point groups are listed in column 2. Column 4 describes one asymmetric unit for the intensity data of each Laue group. Alternative possibilities are separated by dashed lines. The last column shows the fraction of reciprocal space belonging to one asymmetric unit.

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