

Concise intensity statistics of Friedel opposites and classification of the reflections

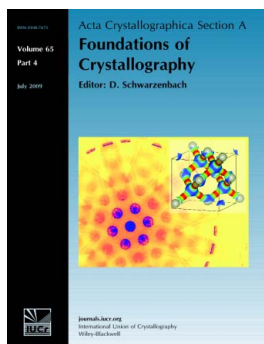
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Concise intensity statistics of Friedel opposites and classification of the reflections

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A previous extensive analysis of the mean-square intensity difference of Friedel opposites [Shmueli *et al.* (2008). *Acta Cryst. A* **64**, 476–483] is here concisely re-examined and confirmed by purely statistical methods. The analysis applies to noncentrosymmetric crystals only. For special reflections and centered lattices both mean-square intensity difference and average intensity of Friedel opposites depend on the centering factor of the crystal lattice and/or on the isotropy subgroup of the reflection. A complete classification of the reflections, based on the above intensity statistics, is presented. It is also shown that the experimentally important Bijvoet ratio is found to depend only on the chemical composition of the unit-cell content and the wavelength of the radiation.

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1. Introduction

A detailed analysis of the mean-square Friedel intensity difference was carried out by Flack & Shmueli (2007) for the simplest triclinic space group $P1$, while assuming the presence of a centrosymmetric substructure. Albeit useful in particular cases, it was by no means obvious that these results are applicable to, or have a bearing on, symmetries other than $P1$. On the contrary, the mean-square Friedel intensity difference depends on the low moments of intensity and these are known to be space-group dependent (*e.g.*, Wilson, 1978). An analysis for all the noncentrosymmetric space groups was therefore carried out. That study (Shmueli *et al.*, 2008), carried out by straightforward algebraic and, in part, probabilistic methods, showed that the mean-square Friedel intensity difference is indeed independent of the space-group symmetry. General and special reflections were considered, and so were primitive and centered lattices.

The present note arrives at these results in a simpler manner while also including a complete point-group-dependent classification of the reflections and relevant examples for its use. It is also shown that the experimentally important Bijvoet ratio (*e.g.* Flack & Bernardinelli, 2008) is independent of the point- and space-group symmetries. We think that this note fills a gap of knowledge on Friedel-difference statistics in a concise and useful style, suitable for applications as well as for future incorporation in crystallographic reference works.

2. Preliminaries

Let g be the number of asymmetric units in the unit cell, G be a lattice-centering factor equal to 1, 2, 3 or 4 for P - and R_{rhomb} -type, A -, B -, C - or I -type, R_{hex} -type or F -type lattices, respectively, N be the number of atoms in the unit cell, N/g be the number of atoms in the asymmetric unit, and let all the atoms be spherical, have only isotropic displacement parameters and be located in general positions, there being no centrosymmetric or any other symmetric substructure. Let $(\mathbf{P}_i, \mathbf{t}_i)$ be the space-group operator generating the i th asymmetric unit from the reference unit (that generated by the identity operator). The structure factor, allowing for resonant scattering, is given by

$$F(\mathbf{h}) = \sum_{j=1}^{N/g} f_j J_j(\mathbf{h}), \quad (1)$$

using the notation of Wilson (1978), with

$$J_j(\mathbf{h}) = \sum_{s=1}^g \exp[2\pi i \mathbf{h}^T (\mathbf{P}_s \mathbf{r}_j + \mathbf{t}_s)], \quad (2)$$

where \mathbf{h}^T is the hkl reflection, general or special, \mathbf{r}_j is the atomic position vector, assumedly general, and $f_j = f_j^{(0)} + f_j' + if_j''$ is the complex atomic scattering factor of the j th atom, where $f_j^{(0)}$ is the scattering factor of the atom assuming that all its electrons behave as if they were free, and f_j' and f_j'' are, respectively, the real and imaginary isotropic parts of the resonant-scattering contribution of the atom.

We recall that in general the following relation between symmetry-related structure factors is valid:

$$F(\mathbf{P}_s^T \mathbf{h}) = F(\mathbf{h}) \exp(-2\pi i \mathbf{h}^T \mathbf{t}_s)$$

(Waser, 1955). Reflection \mathbf{h} is called *special* if there is at least one \mathbf{P}_s , other than identity, for which $\mathbf{P}_s^T \mathbf{h} = \mathbf{h}$. For such a reflection we must have $\exp(-2\pi i \mathbf{h}^T \mathbf{t}_s) = 1$ and this can be so only if $\mathbf{h}^T \mathbf{t}_s$ is an integer.

For each \mathbf{h} there is a subgroup $\mathcal{G}_{\mathbf{h}}$, the operations of which leave \mathbf{h} invariant; it is called the *isotropy subgroup* of \mathbf{h} . If $|\mathcal{G}_{\mathbf{h}}|$ (the order of $\mathcal{G}_{\mathbf{h}}$) is unity, $\mathcal{G}_{\mathbf{h}}$ contains only the identity and \mathbf{h} is then a general reflection. If $|\mathcal{G}_{\mathbf{h}}| > 1$, \mathbf{h} is a special reflection (Stewart & Karle, 1976; Bricogne, 1991). Stewart & Karle (1976) denote the order of the isotropy subgroup by the symbol $\varepsilon_{\mathbf{h}}$.

Another important criterion is the acentric or centric character of a reflection. If at least one of the point-group operators satisfies the relation $\mathbf{P}^T \mathbf{h} = -\mathbf{h}$, the reflection \mathbf{h} is *centric*. If none of the point-group operators satisfies the latter relation, the reflection \mathbf{h} is *acentric*.

These characteristics of the reflection \mathbf{h} will be given for all the noncentrosymmetric point groups in Table 1.

Note that the isotropy subgroup $\mathcal{G}_{\mathbf{h}}$ is a subgroup of the point group of the crystal. The isotropy subgroup is essentially equivalent to the site-symmetry subgroup and its Hermann–Mauguin symbols, as well as its orientations, can be deduced from Table 10.1.2.2 in

Table 1
Classification of the reflections.

See the text for the definition of the symbols.

Point group	h	$ \mathcal{G}_{\mathbf{h}} $	S(sym)	S(h)	$\langle A(\mathbf{h}) \rangle / \Sigma$	$[(D(\mathbf{h})^2) / \rho]^{1/2}$
1	<i>hkl</i>	1	a	ng	<i>G</i>	<i>G</i>
2	<i>hkl</i>	1	a	ng	<i>G</i>	<i>G</i>
	<i>h0l</i>	1	c	ng	<i>G</i>	0
	<i>0k0</i>	2	a	s	<i>2G</i>	<i>2G</i>
<i>m</i>	<i>hkl</i>	1	a	ng	<i>G</i>	<i>G</i>
	<i>h0l</i>	2	a	s	<i>2G</i>	<i>2G</i>
	<i>0k0</i>	1	c	ng	<i>G</i>	0
222	<i>hkl</i>	1	a	ng	<i>G</i>	<i>G</i>
	<i>0kl, h0l, hk0</i>	1	c	ng	<i>G</i>	0
	<i>h00, 0k0, 00l</i>	2	c	s	<i>2G</i>	0
<i>mm2</i>	<i>hkl</i>	1	a	ng	<i>G</i>	<i>G</i>
	<i>0kl, h0l</i>	2	a	s	<i>2G</i>	<i>2G</i>
	<i>hk0</i>	1	c	ng	<i>G</i>	0
	<i>h00, 0k0</i>	2	c	s	<i>2G</i>	0
	<i>00l</i>	4	a	s	<i>4G</i>	<i>4G</i>
4	<i>hkl</i>	1	a	ng	<i>G</i>	<i>G</i>
	<i>hk0</i>	1	c	ng	<i>G</i>	0
	<i>00l</i>	4	a	s	<i>4G</i>	<i>4G</i>
4	<i>hkl</i>	1	a	ng	<i>G</i>	<i>G</i>
	<i>hk0</i>	1	c	ng	<i>G</i>	0
	<i>00l</i>	2	c	s	<i>2G</i>	0
422	<i>hkl</i>	1	a	ng	<i>G</i>	<i>G</i>
	<i>hk0, h0l, hhl</i>	1	c	ng	<i>G</i>	0
	<i>hh0, h00</i>	2	c	s	<i>2G</i>	0
	<i>00l</i>	4	c	s	<i>4G</i>	0
<i>4mm</i>	<i>hkl</i>	1	a	ng	<i>G</i>	<i>G</i>
	<i>hk0</i>	1	c	ng	<i>G</i>	0
	<i>h0l, hhl</i>	2	a	s	<i>2G</i>	<i>2G</i>
	<i>hh0, h00</i>	2	c	s	<i>2G</i>	0
	<i>00l</i>	8	a	s	<i>8G</i>	<i>8G</i>
$\bar{4}2m$	<i>hkl</i>	1	a	ng	<i>G</i>	<i>G</i>
	<i>hk0, h0l</i>	1	c	ng	<i>G</i>	0
	<i>hhl</i>	2	a	s	<i>2G</i>	<i>2G</i>
	<i>hh0, h00</i>	2	c	s	<i>2G</i>	0
	<i>00l</i>	4	c	s	<i>4G</i>	0
$\bar{4}m2$	<i>hkl</i>	1	a	ng	<i>G</i>	<i>G</i>
	<i>hk0, hhl</i>	1	c	ng	<i>G</i>	0
	<i>h0l</i>	2	a	s	<i>2G</i>	<i>2G</i>
	<i>hh0, h00</i>	2	c	s	<i>2G</i>	0
	<i>00l</i>	4	c	s	<i>4G</i>	0
3 (HA)	<i>hkl</i>	1	a	ng	<i>G</i>	<i>G</i>
	<i>00l</i>	3	a	s	<i>3G</i>	<i>3G</i>
3 (RA)	<i>hkl</i>	1	a	ng	<i>G</i>	<i>G</i>
	<i>hhh</i>	3	a	s	<i>3G</i>	<i>3G</i>
312 (HA)	<i>hkl</i>	1	a	ng	<i>G</i>	<i>G</i>
	<i>hhl</i>	1	c	ng	<i>G</i>	0
	<i>h00</i>	2	a	s	<i>2G</i>	<i>2G</i>
	<i>00l</i>	3	c	s	<i>3G</i>	0
321 (HA)	<i>hkl</i>	1	a	ng	<i>G</i>	<i>G</i>
	<i>h0l</i>	1	c	ng	<i>G</i>	0
	<i>hh0</i>	2	a	s	<i>2G</i>	<i>2G</i>
	<i>00l</i>	3	c	s	<i>3G</i>	0
32 (RA)	<i>hkl</i>	1	a	ng	<i>G</i>	<i>G</i>
	<i>hhl</i>	1	c	ng	<i>G</i>	0
	<i>hh0</i>	2	a	s	<i>2G</i>	<i>2G</i>
	<i>hhh</i>	3	c	s	<i>3G</i>	0
3m1 (HA)	<i>hkl</i>	1	a	ng	<i>G</i>	<i>G</i>
	<i>hh0</i>	1	c	ng	<i>G</i>	0
	<i>h0l</i>	2	a	s	<i>2G</i>	<i>2G</i>
	<i>00l</i>	6	a	s	<i>6G</i>	<i>6G</i>
31m (HA)	<i>hkl</i>	1	a	ng	<i>G</i>	<i>G</i>
	<i>h00</i>	1	c	ng	<i>G</i>	0
	<i>hhl</i>	2	a	s	<i>2G</i>	<i>2G</i>
	<i>00l</i>	6	a	s	<i>6G</i>	<i>6G</i>

Table 1 (continued)

Point group	h	$ \mathcal{G}_{\mathbf{h}} $	S(sym)	S(h)	$\langle A(\mathbf{h}) \rangle / \Sigma$	$[(D(\mathbf{h})^2) / \rho]^{1/2}$
3m (RA)	<i>hkl</i>	1	a	g	<i>G</i>	<i>G</i>
	<i>hh0</i>	1	c	ng	<i>G</i>	0
	<i>hhl</i>	2	a	s	<i>2G</i>	<i>2G</i>
	<i>hhh</i>	6	a	s	<i>6G</i>	<i>6G</i>
6	<i>hkl</i>	1	a	g	<i>G</i>	<i>G</i>
	<i>hk0</i>	1	c	ng	<i>G</i>	0
	<i>00l</i>	6	a	s	<i>6G</i>	<i>6G</i>
$\bar{6}$	<i>hkl</i>	1	a	g	<i>G</i>	<i>G</i>
	<i>hk0</i>	2	a	s	<i>2G</i>	<i>2G</i>
	<i>00l</i>	3	c	s	<i>3G</i>	0
622	<i>hkl</i>	1	a	g	<i>G</i>	<i>G</i>
	<i>hk0, h0l, hhl</i>	1	c	ng	<i>G</i>	0
	<i>h00, hh0</i>	2	c	s	<i>2G</i>	0
	<i>00l</i>	6	c	s	<i>6G</i>	0
6mm	<i>hkl</i>	1	a	g	<i>G</i>	<i>G</i>
	<i>hk0</i>	1	c	ng	<i>G</i>	0
	<i>h0l, hhl</i>	2	a	s	<i>2G</i>	<i>2G</i>
	<i>hh0, h00</i>	2	c	s	<i>2G</i>	0
	<i>00l</i>	12	a	s	<i>12G</i>	<i>12G</i>
$\bar{6}m2$	<i>hkl</i>	1	a	ng	<i>G</i>	<i>G</i>
	<i>hhl</i>	1	c	ng	<i>G</i>	0
	<i>hk0, h0l</i>	2	a	s	<i>2G</i>	<i>2G</i>
	<i>hh0</i>	2	c	s	<i>2G</i>	0
	<i>h00</i>	4	a	s	<i>4G</i>	<i>4G</i>
	<i>00l</i>	6	c	s	<i>6G</i>	0
$\bar{6}2m$	<i>hkl</i>	1	a	g	<i>G</i>	<i>G</i>
	<i>h0l</i>	1	c	ng	<i>G</i>	0
	<i>hk0, hhl</i>	2	a	s	<i>2G</i>	<i>2G</i>
	<i>h00</i>	2	c	s	<i>2G</i>	0
	<i>hh0</i>	4	a	s	<i>4G</i>	<i>4G</i>
	<i>00l</i>	6	c	s	<i>6G</i>	0
23	<i>hkl</i>	1	a	g	<i>G</i>	<i>G</i>
	<i>0kl, hh0</i>	1	c	ng	<i>G</i>	0
	<i>h00</i>	2	c	s	<i>2G</i>	0
	<i>hhh</i>	3	a	s	<i>3G</i>	<i>3G</i>
432	<i>hkl</i>	1	a	g	<i>G</i>	<i>G</i>
	<i>hhl, 0kl</i>	1	c	ng	<i>G</i>	0
	<i>hh0</i>	2	c	s	<i>2G</i>	0
	<i>hhh</i>	3	c	s	<i>3G</i>	0
	<i>h00</i>	4	c	s	<i>4G</i>	0
43m	<i>hkl</i>	1	a	g	<i>G</i>	<i>G</i>
	<i>0kl</i>	1	c	ng	<i>G</i>	0
	<i>hhl</i>	2	a	s	<i>2G</i>	<i>2G</i>
	<i>hh0</i>	2	c	s	<i>2G</i>	0
	<i>h00</i>	4	c	s	<i>4G</i>	0
	<i>hhh</i>	6	a	s	<i>6G</i>	<i>6G</i>

International Tables for Crystallography Volume A (Hahn & Klapper, 2002) for the various classes of reflections listed in Table 1.

3. Derivation of the averages

It will be convenient to find first the expressions of the average $\langle |J_j|^2 \rangle$ for the cases of interest. The general expression of this average is

$$\langle |J_j(\mathbf{h})|^2 \rangle = \sum_{s=1}^g \sum_{u=1}^g \langle \exp[2\pi i \mathbf{h}^T (\mathbf{P}_s - \mathbf{P}_u) \mathbf{r}_j] \exp[2\pi i \mathbf{h}^T (\mathbf{t}_s - \mathbf{t}_u)] \rangle. \quad (3)$$

The average for the most general case can be derived by the method of Shmueli *et al.* (2008) but the derivation will be omitted since it leads to the result given by Bertaut (1955, 1956). Bertaut's result, in the present notation, reads

$$\langle |J_j(\mathbf{h})|^2 \rangle = gG|\mathcal{G}_{\mathbf{h}}|. \quad (4)$$

The quantity $|\mathcal{G}_{\mathbf{h}}|$ is also known as the average-intensity multiple; it was first discussed by Wilson (1950) and Rogers (1950), and exten-

sively tabulated by Iwasaki & Ito (1977). Note that since for general reflections $|\mathcal{G}_h| = 1$ and for P - and R_{rhomb} -type lattices $G = 1$, all cases of primitive and centered lattices associated with general or special reflections are contained in equation (4).

The mean-square intensity difference of Friedel opposites, allowing for acentric general or special reflections as well as lattice centering, was derived by Shmueli *et al.* (2008) by a somewhat lengthy method and a more concise rederivation of this quantity by a statistical method, for a special case, was also presented in §4 of the latter reference. We now show that the statistical method used by Shmueli *et al.* (2008) also yields the fully general expression if the equations for the second moment of $|J|$ are taken from equation (4).

The quantity to be evaluated is

$$\langle D(\mathbf{h})^2 \rangle = \langle (|F(\mathbf{h})|^2 - |F(-\mathbf{h})|^2)^2 \rangle \quad (5)$$

$$= \langle |F(\mathbf{h})|^4 \rangle - 2\langle |F(\mathbf{h})|^2 |F(-\mathbf{h})|^2 \rangle + \langle |F(-\mathbf{h})|^4 \rangle. \quad (6)$$

Following Wilson (1978), the fourth moment of $|F(\mathbf{h})|$ is given by

$$\langle |F(\mathbf{h})|^4 \rangle = \sum_{i=1}^{N/g} \sum_{j=1}^{N/g} \sum_{k=1}^{N/g} \sum_{l=1}^{N/g} f_i^* f_j^* f_k f_l \langle J_i(\mathbf{h}) J_j^*(\mathbf{h}) J_k(\mathbf{h}) J_l^*(\mathbf{h}) \rangle \quad (7)$$

$$= \sum_{i=1}^{N/g} |f_i|^4 \langle |J_i(\mathbf{h})|^4 \rangle + 2 \sum_{i=1}^{N/g} \sum_{k=1(i \neq k)}^{N/g} |f_i|^2 |f_k|^2 \langle |J_i(\mathbf{h})|^2 \rangle \langle |J_k(\mathbf{h})|^2 \rangle \quad (8)$$

$$= \sum_{i=1}^{N/g} |f_i|^4 \langle |J_i(\mathbf{h})|^4 \rangle + 2G^2 |\mathcal{G}_h|^2 \sum_{i=1}^N \sum_{k=1(i \neq k)}^N |f_i|^2 |f_k|^2. \quad (9)$$

Equation (9) was obtained from equation (8) by making use of equation (4) as well as of the identity $g \sum_{i=1}^{N/g} = \sum_{i=1}^N$. We can show in a similar manner that

$$\langle |F(-\mathbf{h})|^4 \rangle = \langle |F(\mathbf{h})|^4 \rangle. \quad (10)$$

The remaining term in equation (6) can be calculated in a similar manner and results in

$$-2\langle |F(\mathbf{h})|^2 |F(-\mathbf{h})|^2 \rangle = A_1 + A_2, \quad (11)$$

where

$$A_1 = -2 \sum_{i=1}^{N/g} |f_i|^4 \langle |J_i(\mathbf{h})|^4 \rangle$$

and

$$A_2 = -2G^2 |\mathcal{G}_h|^2 \sum_{i=1}^N \sum_{k=1(i \neq k)}^N [|f_i|^2 |f_k|^2 + \mathcal{R}(f_i^2 f_k^{*2})].$$

If we insert equations (9), (10) and (11) in equation (6) we finally obtain

$$\langle D(\mathbf{h})^2 \rangle = 2G^2 |\mathcal{G}_h|^2 \sum_{i=1}^N \sum_{k=1(i \neq k)}^N [|f_i|^2 |f_k|^2 - \mathcal{R}(f_i^2 f_k^{*2})] \quad (12)$$

$$= 4G^2 |\mathcal{G}_h|^2 \sum_{i=1}^N \sum_{k=1}^N [(f_i^{(0)} + f_i') f_k'' - f_i'' (f_k^{(0)} + f_k')]^2 \quad (13)$$

$$\equiv G^2 |\mathcal{G}_h|^2 \rho, \quad (14)$$

in full agreement with Shmueli *et al.* (2008). Note, however, that for centric reflections $|F(\mathbf{h})| = |F(-\mathbf{h})|$ so $\langle D^2(\mathbf{h}) \rangle = 0$. During this derivation the space-group-dependent fourth moment of $|J(\mathbf{h})|$ appeared in equations (9), (10) and (11) but it canceled out completely, leading to equation (12), which is space-group independent. In the general case, some dependence on symmetry remains in the order of the isotropy subgroup. However, it is not the mean-

square intensity difference which is of importance in experimental work, but rather the Bijvoet ratio (see below).

The average intensity of Friedel opposites can also be derived by the above approach, but we shall use that given by Shmueli *et al.* (2008) as

$$\begin{aligned} A(\mathbf{h}) &= (1/2)(|F(\mathbf{h})|^2 + |F(-\mathbf{h})|^2) \\ &= G |\mathcal{G}_h| \sum_{j=1}^N [(f_j^{(0)} + f_j')^2 + f_j''^2], \end{aligned} \quad (15)$$

$$\equiv G |\mathcal{G}_h| \Sigma. \quad (16)$$

The experimentally important Bijvoet ratio (*e.g.* Flack & Shmueli, 2007) now follows from equations (13) and (15) as

$$\begin{aligned} \chi &= \frac{(\langle D^2(\mathbf{h}) \rangle)^{1/2}}{A(\mathbf{h})} \\ &= \frac{2\{\sum_{i=1}^N \sum_{k=1}^N [(f_i^{(0)} + f_i') f_k'' - f_i'' (f_k^{(0)} + f_k')]^2\}^{1/2}}{\sum_{j=1}^N [(f_j^{(0)} + f_j')^2 + f_j''^2]}. \end{aligned} \quad (17)$$

The Bijvoet ratio thus depends only on the chemical composition of the unit-cell content and the wavelength of the radiation, and is independent of the space-group symmetry and the centering factor of the crystal lattice. However, the Bijvoet ratio given by Flack & Shmueli (2007) was derived only for the triclinic space group $P1$.

4. Classification of the reflections and examples

It follows from equations (13), (14) and (16) and from the redefinition of reflection characteristics that

$$\langle A(\mathbf{h}) \rangle / \Sigma = |\mathcal{G}_h| G \quad \text{for a centric or an acentric reflection} \quad (18)$$

$$\langle [D(\mathbf{h})^2] / \rho \rangle^{1/2} = \begin{cases} |\mathcal{G}_h| G & \text{for an acentric reflection} \\ 0 & \text{for a centric reflection} \end{cases} \quad (19)$$

in agreement with Shmueli *et al.* (2008). While the latter reference presents a tabulation of the above quantities and other characteristics for the point groups 222 and $mm2$, the present Table 1 presents the above quantities for all the noncentrosymmetric point groups. Table 1 contains the average intensity multiples $\langle A(\mathbf{h}) \rangle / \Sigma$ and the important ratio $[\langle D(\mathbf{h})^2 \rangle / \rho]^{1/2}$ for classes of centric and acentric reflections. Column 1 contains the Hermann–Mauguin symbol of the point group; the settings ‘hexagonal axes’ (HA) and ‘rhombohedral axes’ (RA) are indicated. Column 2 contains for each point group the relevant classes of reflections, column 3 contains for each class the order of the isotropy subgroup $|\mathcal{G}_h|$, in column 4 S(sym) is ‘a’ if the reflection is acentric and it is ‘c’ if the reflection is centric, in column 5 S(h) is ‘g’ if the reflection is general and it is ‘s’ if the reflection is special. Columns 6 and 7 contain the values of the expressions given by the left-hand sides of equations (18) and (19), respectively, in terms of the lattice centering factor, G . Table 1 was constructed by consulting Part 10 of *International Tables for Crystallography* Volume A (Hahn & Klapper, 2002) and with the aid of a modified version of program *SPGMIC* (Shmueli, 1984) in which the definitions of general, special, acentric and centric reflections were implemented.

The reflection characteristics in Table 1 are of general value but they also have practical aspects. For example, for all the space groups with point groups 222, $\bar{4}$, 422, 622 and 432 only reflections belonging to the hkl class can be used in application of Friedel differences, since all the other classes are centric and hence their Bijvoet ratios vanish. The same consideration can be applied to centric classes in other point groups listed in Table 1. Notable examples are the $h0l$ class in

point group 2, the $hk0$ class in point group $mm2$ and many others. Thus, the last column of Table 1 is of value in deciding which reflections are likely to give meaningful results in any application relying on measurement of intensity differences between Friedel opposites and is also useful for identifying reflection classes for calibration as the Friedel difference is zero.

References

- Bertaut, E. F. (1955). *Acta Cryst.* **8**, 823–832.
Bertaut, E. F. (1956). *Acta Cryst.* **9**, 322.
- Bricogne, G. (1991). *Acta Cryst.* **A47**, 803–829.
Flack, H. D. & Bernardinelli, G. (2008). *Acta Cryst.* **A64**, 484–493.
Flack, H. D. & Shmueli, U. (2007). *Acta Cryst.* **A63**, 257–265.
Hahn, Th. & Klapper, H. (2002). *International Tables for Crystallography*, Volume A, edited by Th. Hahn, 5th ed., Part 10. Dordrecht: Kluwer Academic Publishers.
Iwasaki, H. & Ito, T. (1977). *Acta Cryst.* **A33**, 227–229.
Rogers, D. (1950). *Acta Cryst.* **3**, 455–464.
Shmueli, U. (1984). *Acta Cryst.* **A40**, 559–567.
Shmueli, U., Schiltz, M. & Flack, H. D. (2008). *Acta Cryst.* **A64**, 476–483.
Stewart, J. M. & Karle, J. (1976). *Acta Cryst.* **A32**, 1005–1007.
Waser, J. (1955). *Acta Cryst.* **8**, 595.
Wilson, A. J. C. (1950). *Acta Cryst.* **3**, 258–261.
Wilson, A. J. C. (1978). *Acta Cryst.* **A34**, 986–994.