

Supplementary material to the article: “Intensity statistics of Friedel opposites” by

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1. Description of Table 3
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The first column presents the standard space group number, as given in the *International Tables for Crystallography*, Volume A. The space group symbol in the second column consists of the Hermann–Mauguin symbol, prefixed by a letter defining the crystal system: the letters *a*, *m* and *o* stand for anorthic (triclinic), monoclinic and orthorhombic respectively. For monoclinic space groups unique *b* axis and standard settings are assumed. For space groups based on an *F* lattice the parities of the reflection indices are designated by *e* (even) and *o* (odd). The quantities listed in the last two columns are defined in the text but will be recalled for clarity. Thus

$$\Sigma = \sum_{j=1}^N (f_j^2 + f''_j{}^2) \quad , \quad \rho = 4 \sum_{j=1}^N \sum_{k=1}^N (f_j f''_k - f''_j f_k)^2,$$

where N is the number of atoms in the unit cell of the nocentrosymmetric space group, A_v is the average reduced intensity and $\langle D^2 \rangle$ is the mean-square reduced intensity difference of Friedel opposites. Reflections not obeying any condition for possible reflection are systematically absent and have $\langle A_v \rangle / \Sigma = \langle D^2 \rangle / \rho = 0$.

Table 3. Average intensity multiples for general and special reflections for low noncentrosymmetric space groups

Space group		Reflections	$\langle A_v \rangle / \Sigma$	$(\langle D^2 \rangle / \rho)^{1/2}$
No.	symbol			
1	<i>aP1</i>	<i>hkl</i>	1	1
3	<i>mP2</i>	<i>hkl</i>	1	1
		<i>h0l</i>	1	0
		<i>0k0</i>	2	2
4	<i>mP2₁</i>	<i>hkl</i>	1	1
		<i>h0l</i>	1	0
		<i>0k0(k = 2n)</i>	2	2
5	<i>mC2</i>	<i>hkl(h + k = 2n)</i>	2	2
		<i>h0l(h = 2n)</i>	2	0
		<i>0k0(k = 2n)</i>	4	4
6	<i>mPm</i>	<i>hkl</i>	1	1
		<i>h0l</i>	2	2
		<i>0k0</i>	1	0
7	<i>mPc</i>	<i>hkl</i>	1	1
		<i>h0l(l = 2n)</i>	2	2
		<i>0k0</i>	1	0
8	<i>mCm</i>	<i>hkl(h + k = 2n)</i>	2	2
		<i>h0l(h = 2n)</i>	4	4
		<i>0k0(k = 2n)</i>	2	0
9	<i>mCc</i>	<i>hkl(h + k = 2n)</i>	2	2
		<i>h0l(h, l = 2n)</i>	4	4
		<i>0k0(k = 2n)</i>	2	0
16	<i>oP222</i>	<i>hkl</i>	1	1
		<i>hk0, 0kl, h0l</i>	1	0
		<i>h00, 0k0, 00l</i>	2	0
17	<i>oP222₁</i>	<i>hkl</i>	1	1
		<i>hk0, 0kl, h0l</i>	1	0
		<i>h00, 0k0, 00l(l = 2n)</i>	2	0
18	<i>oP2₁2₁2</i>	<i>hkl</i>	1	1
		<i>hk0, 0kl, h0l</i>	1	0
		<i>h00(h = 2n), 0k0(k = 2n), 00l</i>	2	0
19	<i>oP2₁2₁2₁</i>	<i>hkl</i>	1	1
		<i>hk0, 0kl, h0l</i>	1	0
		<i>h00(h = 2n), 0k0(k = 2n)</i>	2	0
		<i>00l(l = 2n)</i>	2	0

Table 3. Average intensity multiples for general and special reflections for low noncentrosymmetric space groups (cont.)

Space group		Reflections	$\langle A_v \rangle / \Sigma$	$(\langle D^2 \rangle / \rho)^{1/2}$
No.	symbol			
20	$oC222_1$	$hkl(h+k=2n)$	2	2
		$hk0(h+k=2n), 0kl(k=2n),$ $h0l(h=2n)$	2	0
		$h00(h=2n), 0k0(k=2n),$ $00l(l=2n)$	4	0
21	$oC222$	$hkl(h+k=2n)$	2	2
		$hk0(h+k=2n), 0kl(k=2n),$ $h0l(h=2n)$	2	0
		$h00(h=2n), 0k0(k=2n), 00l$	4	0
22	$oF222$	$hkl(eee, ooo)$	4	4
		$hk0(ee0), 0kl(0ee),$ $h0l(e0e)$	4	0
		$h00(e00), 0k0(0e0), 00l(00e)$	8	0
23	$oI222$	$hkl(h+k+l=2n)$	2	2
		$hk0(h+k=2n), 0kl(k+l=2n),$ $h0l(h+l=2n)$	2	0
		$h00(h=2n), 0k0(k=2n),$ $00l(l=2n)$	4	0
24	$oI2_12_12_1$	$hkl(h+k+l=2n)$	2	2
		$hk0(h+k=2n), 0kl(k+l=2n),$ $h0l(h+l=2n)$	2	0
		$h00(h=2n), 0k0(k=2n),$ $00l(l=2n)$	4	0
25	$oPmm2$	hkl	1	1
		$hk0$	1	0
		$0kl, h0l$	2	2
		$h00, 0k0$	2	0
		$00l$	4	4
26	$oPmc2_1$	hkl	1	1
		$hk0$	1	0
		$0kl, h0l(l=2n)$	2	2
		$h00, 0k0$	2	0
		$00l(l=2n)$	4	4
27	$oPcc2$	hkl	1	1
		$hk0$	1	0
		$0kl(l=2n), h0l(l=2n)$	2	2
		$h00, 0k0$	2	0
		$00l(l=2n)$	4	4

Table 3. Average intensity multiples for general and special reflections for low noncentrosymmetric space groups (cont.)

Space group		Reflections	$\langle A_v \rangle / \Sigma$	$(\langle D^2 \rangle / \rho)^{1/2}$
No.	symbol			
28	<i>oPma2</i>	<i>hkl</i>	1	1
		<i>hk0</i>	1	0
		<i>0kl, h0l(h = 2n)</i>	2	2
		<i>h00(h = 2n), 0k0</i>	2	0
		<i>00l</i>	4	4
29	<i>oPca2₁</i>	<i>hkl</i>	1	1
		<i>hk0</i>	1	0
		<i>0kl(l = 2n), h0l(l = 2n)</i>	2	2
		<i>h00(h = 2n), 0k0</i>	2	0
		<i>00l(l = 2n)</i>	4	4
30	<i>oPnc2</i>	<i>hkl</i>	1	1
		<i>hk0</i>	1	0
		<i>0kl(k + l = 2n), h0l(l = 2n)</i>	2	2
		<i>h00, 0k0(k = 2n)</i>	2	0
		<i>00l(l = 2n)</i>	4	4
31	<i>oPmn2₁</i>	<i>hkl</i>	1	1
		<i>hk0</i>	1	0
		<i>0kl, h0l(h + l = 2n)</i>	2	2
		<i>h00(h = 2n), 0k0</i>	2	0
		<i>00l(l = 2n)</i>	4	4
32	<i>oPba2</i>	<i>hkl</i>	1	1
		<i>hk0</i>	1	0
		<i>0kl(k = 2n), h0l(h = 2n)</i>	2	2
		<i>h00(h = 2n), 0k0(k = 2n)</i>	2	0
		<i>00l</i>	4	4
33	<i>oPna2₁</i>	<i>hkl</i>	1	1
		<i>hk0</i>	1	0
		<i>0kl(k + l = 2n), h0l(h = 2n)</i>	2	2
		<i>h00(h = 2n), 0k0(k = 2n)</i>	2	0
		<i>00l(l = 2n)</i>	4	4
34	<i>oPnn2</i>	<i>hkl</i>	1	1
		<i>hk0</i>	1	0
		<i>0kl(k + l = 2n), h0l(h + l = 2n)</i>	2	2
		<i>h00(h = 2n), 0k0(k = 2n)</i>	2	0
		<i>00l(l = 2n)</i>	4	4

Table 3. Average intensity multiples for general and special reflections for low noncentrosymmetric space groups (cont.)

Space group		Reflections	$\langle A_v \rangle / \Sigma$	$(\langle D^2 \rangle / \rho)^{1/2}$
No.	symbol			
35	<i>oCmm2</i>	<i>hkl</i> ($h + k = 2n$)	2	2
		<i>hk0</i> ($h + k = 2n$)	2	0
		<i>0kl</i> ($k = 2n$), <i>h0l</i> ($h = 2n$)	4	4
		<i>h00</i> ($h = 2n$), <i>0k0</i> ($k = 2n$)	4	0
		<i>00l</i>	8	8
36	<i>oCmc2₁</i>	<i>hkl</i> ($h + k = 2n$)	2	2
		<i>hk0</i> ($h + k = 2n$)	2	0
		<i>0kl</i> ($k = 2n$), <i>h0l</i> ($h, l = 2n$)	4	4
		<i>h00</i> ($h = 2n$), <i>0k0</i> ($k = 2n$)	4	0
		<i>00l</i> ($l = 2n$)	8	8
37	<i>oCcc2</i>	<i>hkl</i> ($h + k = 2n$)	2	2
		<i>hk0</i> ($h + k = 2n$)	2	0
		<i>0kl</i> ($k, l = 2n$), <i>h0l</i> ($h, l = 2n$)	4	4
		<i>h00</i> ($h = 2n$), <i>0k0</i> ($k = 2n$)	4	0
		<i>00l</i> ($l = 2n$)	8	8
38	<i>oAmm2</i>	<i>hkl</i> ($k + l = 2n$)	2	2
		<i>hk0</i> ($k = 2n$)	2	0
		<i>0kl</i> ($k + l = 2n$), <i>h0l</i> ($l = 2n$)	4	4
		<i>h00</i> , <i>0k0</i> ($k = 2n$)	4	0
		<i>00l</i> ($l = 2n$)	8	8
39	<i>oAbm2</i>	<i>hkl</i> ($k + l = 2n$)	2	2
		<i>hk0</i> ($k = 2n$)	2	0
		<i>0kl</i> ($k, l = 2n$), <i>h0l</i> ($l = 2n$)	4	4
		<i>h00</i> , <i>0k0</i> ($k = 2n$)	4	0
		<i>00l</i> ($l = 2n$)	8	8
40	<i>oAma2</i>	<i>hkl</i> ($k + l = 2n$)	2	2
		<i>hk0</i> ($k = 2n$)	2	0
		<i>0kl</i> ($k + l = 2n$), <i>h0l</i> ($h, l = 2n$)	4	4
		<i>h00</i> ($h = 2n$), <i>0k0</i> ($k = 2n$)	4	0
		<i>00l</i> ($l = 2n$)	8	8
41	<i>oAba2</i>	<i>hkl</i> ($k + l = 2n$)	2	2
		<i>hk0</i> ($k = 2n$)	2	0
		<i>0kl</i> ($k, l = 2n$), <i>h0l</i> ($h, l = 2n$)	4	4
		<i>h00</i> ($h = 2n$), <i>0k0</i> ($k = 2n$)	4	0
		<i>00l</i> ($l = 2n$)	8	8
42	<i>oFmm2</i>	<i>hkl</i> (<i>eee</i> , <i>ooo</i>)	4	4
		<i>hk0</i> (<i>ee0</i>)	4	0
		<i>0kl</i> (<i>0ee</i>), <i>h0l</i> (<i>e0e</i>)	8	8
		<i>h00</i> (<i>e00</i>), <i>0k0</i> (<i>0e0</i>)	8	0
		<i>00l</i> (<i>00e</i>)	16	16

Table 3. Average intensity multiples for general and special reflections for low noncentrosymmetric space groups (cont.)

Space group		Reflections	$\langle A_v \rangle / \Sigma$	$(\langle D^2 \rangle / \rho)^{1/2}$
No.	symbol			
43	<i>oFdd2</i>	<i>hkl</i> (<i>eee</i> , <i>ooo</i>)	4	4
		<i>hk0</i> (<i>ee0</i>)	4	0
		<i>0kl</i> (<i>0ee</i> , $k + l = 4n$),		
		<i>h0l</i> (<i>e0e</i> , $h + l = 4n$)	8	8
		<i>h00</i> ($h = 4n$), <i>0k0</i> ($k = 4n$)	8	0
		<i>00l</i> ($l = 4n$)	16	16
44	<i>oImm2</i>	<i>hkl</i> ($h + k + l = 2n$)	2	2
		<i>hk0</i> ($h + k = 2n$)	2	0
		<i>0kl</i> ($k + l = 2n$), <i>h0l</i> ($h + l = 2n$)	4	4
		<i>h00</i> ($h = 2n$), <i>0k0</i> ($k = 2n$)	4	0
		<i>00l</i> ($l = 2n$)	8	8
45	<i>oIba2</i>	<i>hkl</i> ($h + k + l = 2n$)	2	2
		<i>hk0</i> ($h + k = 2n$)	2	0
		<i>0kl</i> ($k, l = 2n$), <i>h0l</i> ($h, l = 2n$)	4	4
		<i>h00</i> ($h = 2n$), <i>0k0</i> ($k = 2n$)	4	0
		<i>00l</i> ($l = 2n$)	8	8
46	<i>oIma2</i>	<i>hkl</i> ($h + k + l = 2n$)	2	2
		<i>hk0</i> ($h + k = 2n$)	2	0
		<i>0kl</i> ($k + l = 2n$), <i>h0l</i> ($h, l = 2n$)	4	4
		<i>h00</i> ($h = 2n$), <i>0k0</i> ($k = 2n$)	4	0
		<i>00l</i> ($l = 2n$)	8	8