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Reflections with phase angle 0 or π in noncentrosymmetric space groups

Il-Hwan Suh *at Department of Physics, Chungnam National University, Taejon 305-764, Korea. E-mail: ihsuh@hanbat.chungnam.ac.kr*

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Abstract

The imaginary parts of structure factors in centrosymmetric space groups disappear so that the phase angle of every reflection is either 0 or π. On the other hand, the phase angles of reflections in noncentrosymmetric space groups can have any value between 0 and 2π. However, some reflections in the noncentrosymmetric space groups under certain conditions behave just like those in the centrosymmetric space groups, which might help to solve the so-called crystallographic phase problem. Reflections with phase angle of either 0 or π in 157 noncentrosymmetric space groups extracted from *International Tables for X-ray Crystallography* (1979), Vol. I (Birmingham: Kynoch Press) are tabulated.

Table 1 shows the noncentrosymmetric space-group numbers and their symbols together with the reflections having phase angles of either 0 or π that belong to monoclinic, orthorhombic, tetragonal, trigonal, hexagonal and cubic systems.

References

International Tables for X-ray Crystallography (1979). Vol. I, edited by N. F. M. Henry & K. Lonsdale, pp. 373–525. Birmingham: Kynoch Press.

Table 1. *Reflections with phase of 0 or π in noncentrosymmetric space groups*

Monoclinic (b as unique axis)		
No. 3 $P2$ $(h0l)$	No. 4 $P2_1$ $(h0l)$	No. 5 $C2$ $(h0l)$
No. 6 Pm $(0k0)$	No. 7 Pc $(0k0)$	No. 8 Cm $(0k0)$
No. 9 Cc $(0k0)$		
Orthorhombic		
No. 16 $P222$ $(hk0)$, $(0kl)$, $(h0l)$	No. 17 $P222_1$ $(0kl)$, $(hk0)$, $(h0l)$ with $l = 2n$	No. 18 $P2_12_12$ $(hk0)$, $(0kl)$ with $k = 2n$, $(h0l)$ with $h = 2n$
No. 19 $P2_12_12_1$ $(0kl)$ with $k = 2n$, $(h0l)$ with $l = 2n$, $(hk0)$ with $h = 2n$	No. 20 $C222_1$ $(h0l)$ with $l = 2n$, $(0kl)$, $(hk0)$	No. 21 $C222$ $(0kl)$, $(h0l)$, $(hk0)$
No. 22 $F222$ $(0kl)$, $(h0l)$, $(hk0)$	No. 23 $I222$ $(0kl)$, $(h0l)$, $(hk0)$	No. 24 $I2_12_12_1$ $(0kl)$ with $l = 2n$, $(h0l)$ with $h = 2n$, $(hk0)$ with $k = 2n$
No. 25 $Pmm2$ $(hk0)$	No. 26 $Pmc2_1$ $(hk0)$	No. 27 $Pcc2$ $(hk0)$
No. 28 $Pma2$ $(hk0)$	No. 29 $Pca2_1$ $(hk0)$	No. 30 $Pnc2$ $(hk0)$
No. 31 $Pmn2_1$ $(hk0)$ with $h = 2n$	No. 32 $Pba2$ $(hk0)$	No. 33 $Pna2_1$ $(hk0)$
No. 34 $Pnn2$ $(hk0)$	No. 35 $Cmm2$ $(hk0)$	No. 36 $Cmc2_1$ $(hk0)$
No. 37 $Ccc2$ $(hk0)$	No. 38 $Amm2$ $(hk0)$	No. 39 $Abm2$ $(hk0)$
No. 40 $Ama2$ $(hk0)$	No. 41 $Aba2$ $(hk0)$	No. 42 $Fmm2$ $(hk0)$
No. 43 $Faa2$ $(hk0)$	No. 44 $Imm2$ $(hk0)$	No. 45 $Iba2$ $(hk0)$
No. 46 $Iam2$ $(hk0)$	No. 48 $Pnnn$ origin at 222 (hkl) with $h = 0$ or $k = 0$ or $l = 0$ or $h+k+l = 2n$	No. 50 $Pban$ origin at 222 (hkl) with $h = 0$ or $k = 0$ or $l = 0$ or $h+k = 2n$
No. 59 $Pmmn$ origin at mmn (hkl) with $h+k = 2n$ or $l = 0$	No. 68 $Ccca$ origin at 222 (hkl) with $h = 0$ or $k = 0$ or $l = 0$ or $h+l = 2n$	No. 70 $Fddd$ origin at 222 (hkl) with $h+k+l = 4n$
Tetragonal		
No. 75 $P4$ $(hk0)$	No. 76 $P4_1$ $(hk0)$	No. 77 $P4_2$ $(hk0)$
No. 78 $P4_3$ $(hk0)$	No. 79 $I4$ $(hk0)$	No. 80 $I4_1$ $(hk0)$
No. 81 $P\bar{4}$ $(hk0)$, $(00l)$	No. 82 $I\bar{4}$ $(hk0)$, $(00l)$	No. 85 $P4/n$ origin at $\bar{4}$ (hkl) with $h = k = 0$ or $l = 0$ or $h+k = 2n$
No. 86 $P4_2/n$ origin at $\bar{4}$ $(hk0)$, $(00l)$, (hkl) with $h+k+l = 2n$	No. 88 $I4_1/a$ origin at $\bar{4}$ (hkl) with $2k+l = 4n$	No. 89 $P422$ (hkl) with $h = 0$ or $k = 0$ or $l = 0$ or $h = \pm k$
No. 90 $P42_12$ $(hk0)$, (hkl) with $h = 0$ and $k = 2n$ (or $k = 0$ and $h = 2n$)	No. 91 $P4_122$ $(0kl)$ with $l = 2n$, (hkl) with $k = 0$ or $l = 0$	No. 92 $P4_12_12$ (hhl) with $l = 2n$, (hkl) with $l = 0$ or $h+k = 0$

Table 1 (*cont.*)

No. 93 $P4_222$ $(0kl)$, $(h0l)$, $(hk0)$	No. 94 $P4_22_12$ $(hk0)$, (hkl) with $h = 0$ and $k+l = 2n$ (or $k = 0$ and $h+l = 2n$)	No. 95 $P4_322$ $(0kl)$ with $l = 2n$, $(h0l)$, $(hk0)$
No. 96 $P4_32_12$ (hhl) with $l = 2n$ (hkl) with $l = 0$ or $h+k = 0$	No. 97 $I422$ $(0kl)$, $(h0l)$, $hk0$	No. 98 $I4_122$ $(hk0)$, (hkl) with $h = \pm k$ and $l = 2n$
No. 99 $P4mm$ $(hk0)$	No. 100 $P4bm$ $(hk0)$	No. 101 $P4_2cm$ $(hk0)$
No. 102 $P4_2nm$ $(hk0)$	No. 103 $P4cc$ $(hk0)$	No. 104 $P4nc$ $(hk0)$
No. 105 $P4_2mc$ $(hk0)$	No. 106 $P4_2bc$ $(hk0)$	No. 107 $I4mm$ $(hk0)$
No. 108 $I4cm$ $(hk0)$	No. 109 $I4_1md$ $(hk0)$	No. 110 $I4_1$cd $(hk0)$
No. 111 $P\bar{4}2m$ $(0kl)$, $(0kl)$, $(hk0)$	No. 112 $P\bar{4}2c$ $(hk0)$, (hkl) with $h = 0$ (or $k = 0$) and $l = 2n$	No. 113 $P\bar{4}2_1m$ $(hk0)$, $(0kl)$ with $k = 2n$, $(h0l)$ with $h = 2n$
No. 114 $P\bar{4}2_1c$ $(hk0)$, $(0kl)$ with $k+l = 2n$, $(h0l)$ with $h+l = 2n$	No. 115 $P\bar{4}m2$ $(hk0)$. (hkl) with $h = \pm k$	No. 116 $P\bar{4}c2$ $(hk0)$, $(00l)$
No. 117 $P\bar{4}b2$ $(hk0)$	No. 118 $P\bar{4}n2$ $(hk0)$, $(00l)$	No. 119 $I\bar{4}m2$ $(hk0)$, (hkl) with $h = \pm k$
No. 120 $I\bar{4}c2$ $(hk0)$, $(00l)$	No. 121 $I\bar{4}2m$ $(0kl)$, $(h0l)$, $(hk0)$	No. 122 $I\bar{4}2d$ $(hk0)$, $(00l)$ with $l = 2n$
No. 125 $P4/nbm$ origin at 422 $(0kl)$, $(h0l)$, $(hk0)$ (hkl) with $h+k = 2n$	No. 126 $P4/nnc$ origin at 422 (hkl) with $h = 0$ or $k = 0$ or $l = 0$ or $h+k+l = 2n$	No. 129 $P4/nmm$ origin at $\bar{4}m2$ $hk0$, hkl with $h+k = 2n$ or $h = \pm k$
No. 130 $P4/ncc$ origin at $\bar{4}$ $(hk0)$, (hkl) with $h+k = 2n$, $(00l)$	No. 133 P_2nbc origin at $\bar{4}$ $(hk0)$, $(0kl)$ with $l = 2n$, $(h0l)$ with $l = 2n$, (hkl) with $h+k+l = 2n$	No. 134 $P4_2/nnm$ origin at $\bar{4}2m$ (hkl) with $h = 0$ or $k = 0$ or $l = 0$ or $h+k+l = 2n$, $(h00)$, $(0k0)$, $(00l)$
No. 137 $P4_2/nmc$ origin at $\bar{4}m2$ $(hk0)$, (hkl) with $h+k+l = 2n$ or $h = \pm k$	No. 138 $P4_2/ncm$ origin at $\bar{4}$ $(hk0)$, (hkl) with $h+k+l = 2n$, $(00l)$	No. 141 $I4_1/amd$ origin at $\bar{4}m2$ (hkl) with $2h+l = 4n$
No. 142 $I4_1/acd$ origin at $\bar{4}$ (hkl) with $2h+l = 4n$		

Trigonal

No. 149 $P312$ (hkl) with $h = k$ or $k = i$ or $i = h$	No. 150 $P321$ (hkl) with $h = -k$ or $k = -i$ or $i = -h$	No. 151 $P3_112$ (hkl) with $l = 3n$ and $h = k$ (or $k = i$ or $i = h$)
No. 152 $P3_121$ (hkl) with $l = 3n$ and $h = -k$ (or $k = -i$ or $i = -h$)	No. 153 $P3_212$ (hkl) with $l = 3n$ and $h = k$ (or $k = i$ or $i = h$)	No. 154 $P3_221$ (hkl) with $l = 3n$ and $h = -k$ (or $k = -i$ or $i = -h$)
No. 155 $R32$ rhombohedral coordinates: (hkl) with $h = k$ or $k = l$ or $l = h$ hexagonal coordinates: (hkl) with $h = -k$ or $k = -i$ or $i = -h$	No. 156 $P3m1$ $(hk0)$ with $h = k$ (or $k = i$ or $i = h$)	No. 157 $P31m$ $(hk0)$ with $h = -k$ (or $k = -i$ or $i = -h$)
No. 158 $P3c1$ $(hk0)$ with $h = k$ (or $k = i$ or $i = h$)	No. 159 $P31c$ $(hk0)$ with $h = -k$ (or $i = -k$ or $h = -i$)	No. 160 $R3m$ rhombohedral coordinates: $(hk0)$ with $h = -k$, $(0kl)$ with $k = -i$, $(h0l)$ with $l = -h$, hexagonal coordinates: $(hk0)$ with $h = k$ or $k = i$ (or $i = h$)
No. 161 $R3c$ rhombohedral coordinates: $(hk0)$ with $h = -k$, $(h0l)$ with $l = -h$, $(0kl)$ with $k = -l$; hexagonal coordinates: $(hk0)$ with $h = k$ (or $k = i$ or $i = h$)		

Hexagonal

No. 168 $P6$ $(hk0)$	No. 169 $P6_1$ $(hk0)$	No. 170 $P6_5$ $(hk0)$
No. 171 $P6_2$ $(hk0)$	No. 172 $P6_4$ $(hk0)$	No. 173 $P6_3$ $(hk0)$
No. 174 $P\bar{6}$ $(00l)$	No. 177 $P622$ $(hk0)$ (hkl) with $h = \pm k$ (or $k = \pm i$ or $i = \pm h$)	No. 178 $P6_122$ $(hk0)$, $(0kl)$, (hkl) with $i = k$ and $l = 2n$
No. 179 $P6_522$ $(hk0)$, (hkl) with $i = k$ and $l = 2n$.	No. 180 $P6_222$ $(hk0)$, (hkl) with $i = k$	No. 181 $P6_422$ $(hk0)$, (hkl) with $i = k$
No. 182 $P6_322$ $(hk0)$, (hkl) with $i = 2n$ and $h = k$ (or $k = i$ or $i = h$)	No. 183 $P6mm$ $(hk0)$	No. 184 $P6cc$ $(hk0)$

Table 1 (*cont.*)

	No. 185 $P6_3cm$ $(hk0)$	No. 186 $P6_3mc$ $(hk0)$	No. 187 $P\bar{6}2m$ (hkl) with $h = k$ (or $k = i$ or $i = h$)
	No. 188 $P\bar{6}c2$ (hkl) with $h = k$ (or $k = i$ or $i = h$)	No. 189 $P\bar{6}2m$ (hkl) with $h = -k$ ($k = -i$ or $i = -h$)	No. 190 $P\bar{6}2c$ (hkl) with $h = -k$ (or $h = -i$ or $i = -k$)
Cubic			
	No. 195 $P23$ $(0kl)$, $(h0l)$, $(hk0)$	No. 196 $F23$ $(0kl)$, $(h0l)$, $(hk0)$	No. 197 $I23$ $(0kl)$, $(h0l)$, $(hk0)$
	No. 198 $P2_13$ $(0kl)$ with $k = 2n$ or $(h0l)$ with $l = 2n$ or $hk0$ with $h = 2n$	No. 199 $I2_13$ $(0kl)$ with $l = 2n$ or $(h0l)$ with $h = 2n$ or $(hk0)$ with $k = 2n$	No. 201 $Pn3$ origin at 23 (hkl) with $h = 0$ or $k = 0$ or $l = 0$ or $h+k+l = 2n$
	No. 203 $Fd3$ origin at 23 (hkl) with $h+k+l = 4n$	No. 207 $P432$ $(0kl)$, $(h0l)$, $(hk0)$, (hkl) with $h = \pm k$ (or $k = \pm l$ or $l = \pm h$)	No. 208 $P4_232$ $(0kl)$, $(h0l)$, $(hk0)$
	No. 209 $F432$ $(0kl)$, $(h0l)$, $(hk0)$	No. 210 $F4_132$ $(0kl)$, $(h0l)$, $(hk0)$	No. 211 $I432$ $(0kl)$, $(h0l)$, $(hk0)$
	No. 212 $P4_332$ $(0kl)$ with $k = 2n$ or $(h0l)$ with $l = 2n$ or $(hk0)$ with $h = 2n$	No. 213 $P4_132$ $(0kl)$ with $k = 2n$, or $(h0l)$ with $l = 2n$ or $(hk0)$ with $h = 2n$	No. 214 $I4_132$ $(h00)$ with $h = 2n$, $(0k0)$ with $k = 2n$, $(00l)$ with $l = 2n$
	No. 215 $P\bar{4}3m$ $(0kl)$, $(h0l)$, $(hk0)$	No. 216 $F\bar{4}3m$ $(0kl)$, $(h0l)$, $(hk0)$	No. 217 $I\bar{4}3m$ (hkl) with $h = 0$ (or $k = 0$ or $l = 0$)
	No. 218 $P\bar{4}3n$ (hkl) with $h = 0$ (or $k = 0$ or $l = 0$)	No. 219 $F\bar{4}3c$ (hkl) with $h = 0$, (or $k = 0$ or $l = 0$)	No. 220 $I\bar{4}3d$ $(h00)$ with $h = 2n$, $(0k0)$ with $k = 2n$, $(00l)$ with $l = 2n$
	No. 222 $Pn\bar{3}n$ origin at 43 (hkl) with $h = 0$ or $k = 0$ or $l = 0$ or $h+k+l = 2n$	No. 224 $Pn\bar{3}m$ origin at $\bar{4}3m$ (hkl) with $h = 0$ or $k = 0$ or $l = 0$ or $h+k+l = 2n$	No. 227 $Fd\bar{3}m$ origin at $\bar{4}3m$ (hkl) with $h+k+l = 4n$
	No. 228 $Fd\bar{3}c$ origin at 23 (hkl) with $h+k+l = 4n$		