Space Group Encoding

This file contains the conversion tables for a compact space group encoding scheme. Table 1 lists the point symmetry parts of the 14 basic matrices, and Table 2 lists the conversions for the components of translation vectors. The remaining tables contain the generator strings for all 230 space groups. These tables should be used along with the information in section 10.7 (page 252) of the text book.[1]

Table 1: Explicit point symmetry matrices for the 14 matrices used to encode the space group generators.

$a = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$b = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$c = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$
$d = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	$e = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$f = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$
$g = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$h = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$i = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$
$j = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$k = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$l = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
$m = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$n = \begin{pmatrix} 0 & -1 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	

Table 2: Conversions for the components of translation vectors in the space group encoding scheme.

$A = \frac{1}{6}$	$B = \frac{1}{4}$	$C = \frac{1}{3}$	$D = \frac{1}{2}$	$E = \frac{2}{3}$	$F = \frac{3}{4}$
$G = \frac{5}{6}$	$O = 0$	$X = -\frac{3}{8}$	$Y = -\frac{1}{4}$	$Z = -\frac{1}{8}$	

[1] Four errors in the generator strings (for space groups 90, 107, 108, and 214) were pointed out by Matthew G. O'Brien and were corrected in this document on 9/25/2011.

Table 3: Generator strings for the 230 space groups.

Space Group	Generators	Space Group	Generators
1–**P1** (C_1^1)	*000*	2–**P$\bar{1}$** (C_i^1)	*100*
3–**P2** (C_2^1)	*01cOOO0*	4–**P2$_1$** (C_2^2)	*01cODO0*
5–**C2** (C_2^3)	*02aDDOcOOO0*	6–**Pm** (C_s^1)	*01jOOO0*
7–**Pc** (C_s^2)	*01jOOD0*	8–**Cm** (C_s^3)	*02aDDOjOOO0*
9–**Cc** (C_s^4)	*02aDDOjOOD0*	10–**P2/m** (C_{2h}^1)	*11cOOO0*
11–**P2$_1$/m** (C_{2h}^2)	*11cODO0*	12–**C2/m** (C_{2h}^3)	*12aDDOcOOO0*
13–**P2/c** (C_{2h}^4)	*11cOOD0*	14–**P2$_1$/c** (C_{2h}^5)	*11cODD0*
15–**C2/c** (C_{2h}^6)	*12aDDOcOOD0*	16–**P222** (D_2^1)	*02bOOOcOOO0*
17–**P222$_1$** (D_2^2)	*02bOODcOOD0*	18–**P2$_1$2$_1$2** (D_2^3)	*02bOOOcDDO0*
19–**P2$_1$2$_1$2$_1$** (D_2^4)	*02bDODcODD0*	20–**C222$_1$** (D_2^5)	*03aDDObOODcOOD0*
21–**C222** (D_2^6)	*03aDDObOOOcOOO0*	22–**F222** (D_2^7)	*04aODDaDODbOOOcOOO0*
23–**I222** (D_2^8)	*03aDDDbOOOcOOO0*	24–**I2$_1$2$_1$2$_1$** (D_2^9)	*03aDDDbDODcODD0*
25–**Pmm2** (C_{2v}^1)	*02bOOOjOOO0*	26–**Pmc2$_1$** (C_{2v}^2)	*02bOODjOOD0*
27–**Pcc2** (C_{2v}^3)	*02bOOOjOOD0*	28–**Pma2** (C_{2v}^4)	*02bOOOjDOO0*
29–**Pca2$_1$** (C_{2v}^5)	*02bOODjDOO0*	30–**Pnc2** (C_{2v}^6)	*02bOOOjODD0*
31–**Pmn2$_1$** (C_{2v}^7)	*02bDODjDOD0*	32–**Pba2** (C_{2v}^8)	*02bOOOjDDO0*
33–**Pna2$_1$** (C_{2v}^9)	*02bOODjDDO0*	34–**Pnn2** (C_{2v}^{10})	*02bOOOjDDD0*
35–**Cmm2** (C_{2v}^{11})	*03aDDObOOOjOOO0*	36–**Cmc2$_1$** (C_{2v}^{12})	*03aDDObOODjOOD0*
37–**Ccc2** (C_{2v}^{13})	*03aDDObOOOjOOD0*	38–**Amm2** (C_{2v}^{14})	*03aODDbOOOjOOO0*
39–**Abm2** (C_{2v}^{15})	*03aODDbOOOcODO0*	40–**Ama2** (C_{2v}^{16})	*03aODDbOOOjDOO0*
41–**Aba2** (C_{2v}^{17})	*03aODDbOOOjDDO0*	42–**Fmm2** (C_{2v}^{18})	*04aODDaDODbOOOjOOO0*
43–**Fdd2** (C_{2v}^{19})	*04aODDaDODbOOOjBBB0*	44–**Imm2** (C_{2v}^{20})	*03aDDDbOOOjOOO0*
45–**Iba2** (C_{2v}^{21})	*03aDDDbOOOjDDO0*	46–**Ima2** (C_{2v}^{22})	*03aDDDbOOOjDOO0*
47–**Pmmm** (D_{2h}^1)	*12bOOOcOOO0*	48–**Pnnn** (D_{2h}^2)	*03bOOOcOOOhDDD1BBB*
49–**Pccm** (D_{2h}^3)	*12bOOOcOOD0*	50–**Pban** (D_{2h}^4)	*03bOOOcOOOhDDO1BBO*
51–**Pmma** (D_{2h}^5)	*12bDOOcOOO0*	52–**Pnna** (D_{2h}^6)	*12bDOOcDDD0*
53–**Pmna** (D_{2h}^7)	*12bDODcDOD0*	54–**Pcca** (D_{2h}^8)	*12bDOOcOOD0*
55–**Pbam** (D_{2h}^9)	*12bOOOcDDO0*	56–**Pccn** (D_{2h}^{10})	*12bDDOcODD0*
57–**Pbcm** (D_{2h}^{11})	*12bOODcODD0*	58–**Pnnm** (D_{2h}^{12})	*12bOOOcDDD0*
59–**Pmmn** (D_{2h}^{13})	*03bOOOcDDOhDDO1BBO*	60–**Pbcn** (D_{2h}^{14})	*12bDDDcOOD0*
61–**Pbca** (D_{2h}^{15})	*12bDODcODD0*	62–**Pnma** (D_{2h}^{16})	*12bDODcODO0*
63–**Cmcm** (D_{2h}^{17})	*13aDDObOODcOOD0*	64–**Cmca** (D_{2h}^{18})	*13aDDObODDcODD0*
65–**Cmmm** (D_{2h}^{19})	*13aDDObOOOcOOO0*	66–**Cccm** (D_{2h}^{20})	*13aDDObOOOcOOD0*
67–**Cmma** (D_{2h}^{21})	*13aDDObODOcODO0*	68–**Ccca** (D_{2h}^{22})	*04aDDObDDOcOOOhODD1OBB*
69–**Fmmm** (D_{2h}^{23})	*14aODDaDODbOOOcOOO0*	70–**Fddd** (D_{2h}^{24})	*05aODDaDODbOOOcOOOhBBB1ZZZ*
71–**Immm** (D_{2h}^{25})	*13aDDDbOOOcOOO0*	72–**Ibam** (D_{2h}^{26})	*13aDDDbOOOcDDO0*
73–**Ibca** (D_{2h}^{27})	*13aDDDbDODcODD0*	74–**Imma** (D_{2h}^{28})	*13aDDDbODOcODO0*
75–**P4** (C_4^1)	*02bOOOgOOO0*	76–**P4$_1$** (C_4^2)	*02bOODgOOB0*
77–**P4$_2$** (C_4^3)	*02bOOOgOOD0*	78–**P4$_3$** (C_4^4)	*02bOODgOOF0*
79–**I4** (C_4^5)	*03aDDDbOOOgOOO0*	80–**I4$_1$** (C_4^6)	*03aDDDbDDDgODB0*

Table 3: Generator strings for the 230 space groups (continued).

Space Group	Generators	Space Group	Generators
81–**P$\bar{4}$** (S_4^1)	*02bOOOmOOO0*	82–**I$\bar{4}$** (S_4^2)	*03aDDDbOOOmOOO0*
83–**P4/m** (C_{4h}^1)	*12bOOOgOOO0*	84–**P4$_2$/m** (C_{4h}^2)	*12bOOOgOOD0*
85–**P4/n** (C_{4h}^3)	*03bOOOgDDOhDDO1YBO*	86–**P4$_2$/n** (C_{4h}^4)	*03bOOOgDDDhDDD1YYY*
87–**I4/m** (C_{4h}^5)	*13aDDDbOOOgOOO0*	88–**I4$_1$/a** (C_{4h}^6)	*04aDDDbDDDgODBhODB1OYZ*
89–**P422** (D_4^1)	*03bOOOgOOOcOOO0*	90–**P42$_1$2** (D_4^2)	*03bOOOgDDOcDDO0*
91–**P4$_1$22** (D_4^3)	*03bOODgOOBcOOO0*	92–**P4$_1$2$_1$2** (D_4^4)	*03bOODgDDBcDDB0*
93–**P4$_2$22** (D_4^5)	*03bOOOgOODcOOO0*	94–**P4$_2$2$_1$2** (D_4^6)	*03bOOOgDDDcDDD0*
95–**P4$_3$22** (D_4^7)	*03bOODgOOFcOOO0*	96–**P4$_3$2$_1$2** (D_4^8)	*03bOODgDDFcDDF0*
97–**I422** (D_4^9)	*04aDDDbOOOgOOOcOOO0*	98–**I4$_1$22** (D_4^{10})	*04aDDDbDDDgODBcDOF0*
99–**P4mm** (C_{4v}^1)	*03bOOOgOOOjOOO0*	100–**P4bm** (C_{4v}^2)	*03bOOOgOOOjDDO0*
101–**P4$_2$cm** (C_{4v}^3)	*03bOOOgOODjOOD0*	102–**P4$_2$nm** (C_{4v}^4)	*03bOOOgDDDjDDD0*
103–**P4cc** (C_{4v}^5)	*03bOOOgOOOjOOD0*	104–**P4nc** (C_{4v}^6)	*03bOOOgOOOjDDD0*
105–**P4$_2$mc** (C_{4v}^7)	*03bOOOgOODjOOO0*	106–**P4$_2$bc** (C_{4v}^8)	*03bOOOgOODjDDO0*
107–**I4mm** (C_{4v}^9)	*04aDDDbOOOgOOOjOOO0*	108–**I4cm** (C_{4v}^{10})	*04aDDDbOOOgOOOjOOD0*
109–**I4$_1$md** (C_{4v}^{11})	*04aDDDbDDDgODBjOOO0*	110–**I4$_1$cd** (C_{4v}^{12})	*04aDDDbDDDgODBjOOD0*
111–**P$\bar{4}$2m** (D_{2d}^1)	*03bOOOmOOOcOOO0*	112–**P$\bar{4}$2c** (D_{2d}^2)	*03bOOOmOOOcOOD0*
113–**P$\bar{4}$2$_1$m** (D_{2d}^3)	*03bOOOmOOOcDDO0*	114–**P$\bar{4}$2$_1$c** (D_{2d}^4)	*03bOOOmOOOcDDD0*
115–**P$\bar{4}$m2** (D_{2d}^5)	*03bOOOmOOOjOOO0*	116–**P$\bar{4}$c2** (D_{2d}^6)	*03bOOOmOOOjOOD0*
117–**P$\bar{4}$b2** (D_{2d}^7)	*03bOOOmOOOjDDO0*	118–**P$\bar{4}$n2** (D_{2d}^8)	*03bOOOmOOOjDDD0*
119–**I$\bar{4}$m2** (D_{2d}^9)	*04aDDDbOOOmOOOjOOO0*	120–**I$\bar{4}$c2** (D_{2d}^{10})	*04aDDDbOOOmOOOjOOD0*
121–**I$\bar{4}$2m** (D_{2d}^{11})	*04aDDDbOOOmOOOcOOO0*	122–**I$\bar{4}$2d** (D_{2d}^{12})	*04aDDDbOOOmOOOcDOF0*
123–**P4/mmm** (D_{4h}^1)	*13bOOOgOOOcOOO0*	124–**P4/mcc** (D_{4h}^2)	*13bOOOgOOOcOOD0*
125–**P4/nbm** (D_{4h}^3)	*04bOOOgOOOcOOOhDDO1YYO*	126–**P4/nnc** (D_{4h}^4)	*04bOOOgOOOcOOOhDDD1YYY*
127–**P4/mbm** (D_{4h}^5)	*13bOOOgOOOcDDO0*	128–**P4/mnc** (D_{4h}^6)	*13bOOOgOOOcDDD0*
129–**P4/nmm** (D_{4h}^7)	*04bOOOgDDOcDDOhDDO1YBO*	130–**P4/ncc** (D_{4h}^8)	*04bOOOgDDOcDDDhDDO1YBO*
131–**P4$_2$/mmc** (D_{4h}^9)	*13bDDOgDOOcODD0*	132–**P4$_2$/mcm** (D_{4h}^{10})	*13bOOOgOODcOOD0*
133–**P4$_2$/nbc** (D_{4h}^{11})	*04bOOOgDDDcOODhDDD1YBY*	134–**P4$_2$/nnm** (D_{4h}^{12})	*04bOOOgDDDcOOOhDDD1YBY*
135–**P4$_2$/mbc** (D_{4h}^{13})	*13bOOOgOODcDDO0*	136–**P4$_2$/mnm** (D_{4h}^{14})	*13bOOOgDDDcDDD0*
137–**P4$_2$/nmc** (D_{4h}^{15})	*04bOOOgDDDcDDDhDDD1YBY*	138–**P4$_2$/ncm** (D_{4h}^{16})	*04bOOOgDDDcDDOhDDD1YBY*
139–**I4/mmm** (D_{4h}^{17})	*14aDDDbOOOgOOOcOOO0*	140–**I4/mcm** (D_{4h}^{18})	*14aDDDbOOOgOOOcOOD0*
141–**I4$_1$/amd** (D_{4h}^{19})	*05aDDDbDDDgODBcDOFhODB1OBZ*	142–**I4$_1$/acd** (D_{4h}^{20})	*05aDDDbDDDgODBcDOBhODB1OBZ*
143–**P3** (C_3^1)	*01nOOO0*	144–**P3$_1$** (C_3^2)	*01nOOC0*
145–**P3$_2$** (C_3^3)	*01nOOE0*	146–**R3** (C_3^4)	*02aECCnOOO0*
147–**P$\bar{3}$** (C_{3i}^1)	*11nOOO0*	148–**R$\bar{3}$** (C_{3i}^2)	*12aECCnOOO0*
149–**P312** (D_3^1)	*02nOOOfOOO0*	150–**P321** (D_3^2)	*02nOOOeOOO0*
151–**P3$_1$12** (D_3^3)	*02nOOCfOOE0*	152–**P3$_1$21** (D_3^4)	*02nOOCeOOO0*
153–**P3$_2$12** (D_3^5)	*02nOOEfOOC0*	154–**P3$_2$21** (D_3^6)	*02nOOEeOOO0*
155–**R32** (D_3^7)	*03aECCnOOOeOOO0*	156–**P3m1** (C_{3v}^1)	*02nOOOkOOO0*
157–**P31m** (C_{3v}^2)	*02nOOOlOOO0*	158–**P3c1** (C_{3v}^3)	*02nOOOkOOD0*
159–**P31c** (C_{3v}^4)	*02nOOOlOOD0*	160–**R3m** (C_{3v}^5)	*03aECCnOOOkOOO0*

Table 3: Generator strings for the 230 space groups (continued).

Space Group	Generators	Space Group	Generators
161–**R3c** (C_{3v}^{6})	*03aECCnOOOkOOD0*	162–**P$\bar{3}$1m** (D_{3d}^{1})	*12nOOOfOOO0*
163–**P$\bar{3}$1c** (D_{3d}^{2})	*12nOOOfOOD0*	164–**P$\bar{3}$m1** (D_{3d}^{3})	*12nOOOeOOO0*
165–**P$\bar{3}$c1** (D_{3d}^{4})	*12nOOOeOOD0*	166–**R$\bar{3}$m** (D_{3d}^{5})	*13aECCnOOOeOOO0*
167–**R$\bar{3}$c** (D_{3d}^{6})	*13aECCnOOOeOOD0*	168–**P6** (C_{6}^{1})	*02nOOObOOO0*
169–**P6$_1$** (C_{6}^{2})	*02nOOCbOOD0*	170–**P6$_5$** (C_{6}^{3})	*02nOOEbOOD0*
171–**P6$_2$** (C_{6}^{4})	*02nOOEbOOO0*	172–**P6$_4$** (C_{6}^{5})	*02nOOCbOOO0*
173–**P6$_3$** (C_{6}^{6})	*02nOOObOOD0*	174–**P$\bar{6}$** (C_{3h}^{1})	*02nOOOiOOO0*
175–**P6/m** (C_{6h}^{1})	*12nOOObOOO0*	176–**P6$_3$/m** (C_{6h}^{2})	*12nOOObOOD0*
177–**P622** (D_{6}^{1})	*03nOOObOOOeOOO0*	178–**P6$_1$22** (D_{6}^{2})	*03nOOCbOODeOOC0*
179–**P6$_5$22** (D_{6}^{3})	*03nOOEbOODeOOE0*	180–**P6$_2$22** (D_{6}^{4})	*03nOOEbOOOeOOE0*
181–**P6$_4$22** (D_{6}^{5})	*03nOOCbOOOeOOC0*	182–**P6$_3$22** (D_{6}^{6})	*03nOOObOODeOOO0*
183–**P6mm** (C_{6v}^{1})	*03nOOObOOOkOOO0*	184–**P6cc** (C_{6v}^{2})	*03nOOObOOOkOOD0*
185–**P6$_3$cm** (C_{6v}^{3})	*03nOOObOODkOOD0*	186–**P6$_3$mc** (C_{6v}^{4})	*03nOOObOODkOOO0*
187–**P$\bar{6}$m2** (D_{3h}^{1})	*03nOOOiOOOkOOO0*	188–**P$\bar{6}$c2** (D_{3h}^{2})	*03nOOOiOODkOOD0*
189–**P$\bar{6}$2m** (D_{3h}^{3})	*03nOOOiOOOeOOO0*	190–**P$\bar{6}$2c** (D_{3h}^{4})	*03nOOOiOODeOOO0*
191–**P6/mmm** (D_{6h}^{1})	*13nOOObOOOeOOO0*	192–**P6/mcc** (D_{6h}^{2})	*13nOOObOOOeOOD0*
193–**P6$_3$/mcm** (D_{6h}^{3})	*13nOOObOODeOOD0*	194–**P6$_3$/mmc** (D_{6h}^{4})	*13nOOObOODeOOO0*
195–**P23** (T^{1})	*03bOOOcOOOdOOO0*	196–**F23** (T^{2})	*05aODDaDODbOOOcOOOdOOO0*
197–**I23** (T^{3})	*04aDDDbOOOcOOOdOOO0*	198–**P2$_1$3** (T^{4})	*03bDODcODDdOOO0*
199–**I2$_1$3** (T^{5})	*04aDDDbDODcODDdOOO0*	200–**Pm$\bar{3}$** (T_{h}^{1})	*13bOOOcOOOdOOO0*
201–**Pn$\bar{3}$** (T_{h}^{2})	*04bOOOcOOOdOOOhDDD1YYY*	202–**Fm$\bar{3}$** (T_{h}^{3})	*15aODDaDODbOOOcOOOdOOO0*
203–**Fd$\bar{3}$** (T_{h}^{4})	*06aODDaDODbOOOcOOOdOOOhBBB1ZZZ*	204–**Im$\bar{3}$** (T_{h}^{5})	*14aDDDbOOOcOOOdOOO0*
205–**Pa$\bar{3}$** (T_{h}^{6})	*13bDODcODDdOOO0*	206–**Ia$\bar{3}$** (T_{h}^{7})	*14aDDDbDODcODDdOOO0*
207–**P432** (O^{1})	*04bOOOcOOOdOOOeOOO0*	208–**P4$_2$32** (O^{2})	*04bOOOcOOOdOOOeDDD0*
209–**F432** (O^{3})	*06aODDaDODbOOOcOOOdOOOeOOO0*	210–**F4$_1$32** (O^{4})	*06aODDaDODbODDcDDOdOOOeFBF0*
211–**I432** (O^{5})	*05aDDDbOOOcOOOdOOOeOOO0*	212–**P4$_3$32** (O^{6})	*04bDODcODDdOOOeBFF0*
213–**P4$_1$32** (O^{7})	*04bDODcODDdOOOeFBB0*	214–**I4$_1$32** (O^{8})	*05aDDDbDODcODDdOOOeFBB0*
215–**P$\bar{4}$3m** (T_{d}^{1})	*04bOOOcOOOdOOOlOOO0*	216–**F$\bar{4}$3m** (T_{d}^{2})	*06aODDaDODbOOOcOOOdOOOlOOO0*
217–**I$\bar{4}$3m** (T_{d}^{3})	*05aDDDbOOOcOOOdOOOlOOO0*	218–**P$\bar{4}$3n** (T_{d}^{4})	*04bOOOcOOOdOOOlDDD0*
219–**F$\bar{4}$3c** (T_{d}^{5})	*06aODDaDODbOOOcOOOdOOOlDDD0*	220–**I$\bar{4}$3d** (T_{d}^{6})	*05aDDDbDODcODDdOOOlBBB0*
221–**Pm$\bar{3}$m** (O_{h}^{1})	*14bOOOcOOOdOOOeOOO0*	222–**Pn$\bar{3}$n** (O_{h}^{2})	*14bDDOcDODdOOOeOOD1YYY*
223–**Pm$\bar{3}$n** (O_{h}^{3})	*14bOOOcOOOdOOOeDDD0*	224–**Pn$\bar{3}$m** (O_{h}^{4})	*05bOOOcOOOdOOOeDDDhDDD1YYY*
225–**Fm$\bar{3}$m** (O_{h}^{5})	*16aODDaDODbOOOcOOOdOOOeOOO0*	226–**Fm$\bar{3}$c** (O_{h}^{6})	*16aODDaDODbOOOcOOOdOOOeDDD0*
227–**Fd$\bar{3}$m** (O_{h}^{7})	*07aODDaDODbODDcDDOdOOOeFBFhBBB1ZZZ*	228–**Fd$\bar{3}$c** (O_{h}^{8})	*07aODDaDODbODDcDDOdOOOeFBFhFFF1XXX*
229–**Im$\bar{3}$m** (O_{h}^{9})	*15aDDDbOOOcOOOdOOOeOOO0*	230–**Ia$\bar{3}$d** (O_{h}^{10})	*15aDDDbDODcODDdOOOeFBB0*