

MSG No. 188.216 $P\bar{6}c21'$ [Type II, hexagonal]

Table 1: Wyckoff site: 2a, site symmetry: 3.21'

No.	position	mapping
1	[0, 0, 0]	[1,2,3,4,5,6,13,14,15,16,17,18]
2	[0, 0, $\frac{1}{2}$]	[7,8,9,10,11,12,19,20,21,22,23,24]

Table 2: Wyckoff site: 2b, site symmetry: -6..1'

No.	position	mapping
1	[0, 0, $\frac{1}{4}$]	[1,2,3,7,8,9,13,14,15,19,20,21]
2	[0, 0, $\frac{3}{4}$]	[4,5,6,10,11,12,16,17,18,22,23,24]

Table 3: Wyckoff site: 2c, site symmetry: 3.21'

No.	position	mapping
1	[$\frac{1}{3}$, $\frac{2}{3}$, 0]	[1,2,3,4,5,6,13,14,15,16,17,18]
2	[$\frac{1}{3}$, $\frac{2}{3}$, $\frac{1}{2}$]	[7,8,9,10,11,12,19,20,21,22,23,24]

Table 4: Wyckoff site: 2d, site symmetry: -6..1'

No.	position	mapping
1	[$\frac{1}{3}$, $\frac{2}{3}$, $\frac{1}{4}$]	[1,2,3,7,8,9,13,14,15,19,20,21]
2	[$\frac{1}{3}$, $\frac{2}{3}$, $\frac{3}{4}$]	[4,5,6,10,11,12,16,17,18,22,23,24]

Table 5: Wyckoff site: 2e, site symmetry: 3.21'

No.	position	mapping
1	[$\frac{2}{3}$, $\frac{1}{3}$, 0]	[1,2,3,4,5,6,13,14,15,16,17,18]
2	[$\frac{2}{3}$, $\frac{1}{3}$, $\frac{1}{2}$]	[7,8,9,10,11,12,19,20,21,22,23,24]

Table 6: Wyckoff site: 2f, site symmetry: -6..1'

No.	position	mapping
1	[$\frac{2}{3}$, $\frac{1}{3}$, $\frac{1}{4}$]	[1,2,3,7,8,9,13,14,15,19,20,21]
2	[$\frac{2}{3}$, $\frac{1}{3}$, $\frac{3}{4}$]	[4,5,6,10,11,12,16,17,18,22,23,24]

Table 7: Wyckoff site: 4g, site symmetry: 3..1'

No.	position	mapping
1	[0, 0, z]	[1,2,3,13,14,15]
2	[0, 0, -z]	[4,5,6,16,17,18]
3	[0, 0, $\frac{1}{2}$ - z]	[7,8,9,19,20,21]
4	[0, 0, $z + \frac{1}{2}$]	[10,11,12,22,23,24]

Table 8: Wyckoff site: 4h, site symmetry: 3..1'

No.	position	mapping
1	[$\frac{1}{3}$, $\frac{2}{3}$, z]	[1,2,3,13,14,15]
2	[$\frac{1}{3}$, $\frac{2}{3}$, -z]	[4,5,6,16,17,18]
3	[$\frac{1}{3}$, $\frac{2}{3}$, $\frac{1}{2}$ - z]	[7,8,9,19,20,21]
4	[$\frac{1}{3}$, $\frac{2}{3}$, $z + \frac{1}{2}$]	[10,11,12,22,23,24]

Table 9: Wyckoff site: 4i, site symmetry: 3..1'

No.	position	mapping
1	[$\frac{2}{3}$, $\frac{1}{3}$, z]	[1,2,3,13,14,15]
2	[$\frac{2}{3}$, $\frac{1}{3}$, -z]	[4,5,6,16,17,18]
3	[$\frac{2}{3}$, $\frac{1}{3}$, $\frac{1}{2}$ - z]	[7,8,9,19,20,21]
4	[$\frac{2}{3}$, $\frac{1}{3}$, $z + \frac{1}{2}$]	[10,11,12,22,23,24]

Table 10: Wyckoff site: 6j, site symmetry: ..21'

No.	position	mapping
1	[x, -x, 0]	[1,6,13,18]
2	[x, 2x, 0]	[2,4,14,16]
3	[-2x, -x, 0]	[3,5,15,17]
4	[-2x, -x, $\frac{1}{2}$]	[7,10,19,22]
5	[x, -x, $\frac{1}{2}$]	[8,11,20,23]
6	[x, 2x, $\frac{1}{2}$]	[9,12,21,24]

Table 11: Wyckoff site: 6k, site symmetry: m..1'

No.	position	mapping
1	[x, y, $\frac{1}{4}$]	[1,8,13,20]
2	[-y, x - y, $\frac{1}{4}$]	[2,9,14,21]

continued ...

Table 11

No.	position	mapping
3	$[-x + y, -x, \frac{1}{4}]$	[3, 7, 15, 19]
4	$[x, x - y, \frac{3}{4}]$	[4, 12, 16, 24]
5	$[-x + y, y, \frac{3}{4}]$	[5, 10, 17, 22]
6	$[-y, -x, \frac{3}{4}]$	[6, 11, 18, 23]

Table 12: Wyckoff site: 121, site symmetry: 11'

No.	position	mapping
1	$[x, y, z]$	[1, 13]
2	$[-y, x - y, z]$	[2, 14]
3	$[-x + y, -x, z]$	[3, 15]
4	$[x, x - y, -z]$	[4, 16]
5	$[-x + y, y, -z]$	[5, 17]
6	$[-y, -x, -z]$	[6, 18]
7	$[-x + y, -x, \frac{1}{2} - z]$	[7, 19]
8	$[x, y, \frac{1}{2} - z]$	[8, 20]
9	$[-y, x - y, \frac{1}{2} - z]$	[9, 21]
10	$[-x + y, y, z + \frac{1}{2}]$	[10, 22]
11	$[-y, -x, z + \frac{1}{2}]$	[11, 23]
12	$[x, x - y, z + \frac{1}{2}]$	[12, 24]