

MSG No. 188.219 $P\bar{6}c'2'$ [Type III, hexagonal]

Table 1: Wyckoff site: 2a, site symmetry: 3.2'

No.	position	mapping
1	[0, 0, 0]	[1,2,3,7,8,9]
2	[0, 0, $\frac{1}{2}$]	[4,5,6,10,11,12]

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

No.	position	mapping
1	[0, 0, $\frac{1}{4}$]	[1,2,3,4,5,6]
2	[0, 0, $\frac{3}{4}$]	[7,8,9,10,11,12]

Table 3: Wyckoff site: 2c, site symmetry: 3.2'

No.	position	mapping
1	[$\frac{1}{3}$, $\frac{2}{3}$, 0]	[1,2,3,7,8,9]
2	[$\frac{1}{3}$, $\frac{2}{3}$, $\frac{1}{2}$]	[4,5,6,10,11,12]

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

No.	position	mapping
1	[$\frac{1}{3}$, $\frac{2}{3}$, $\frac{1}{4}$]	[1,2,3,4,5,6]
2	[$\frac{1}{3}$, $\frac{2}{3}$, $\frac{3}{4}$]	[7,8,9,10,11,12]

Table 5: Wyckoff site: 2e, site symmetry: 3.2'

No.	position	mapping
1	[$\frac{2}{3}$, $\frac{1}{3}$, 0]	[1,2,3,7,8,9]
2	[$\frac{2}{3}$, $\frac{1}{3}$, $\frac{1}{2}$]	[4,5,6,10,11,12]

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

No.	position	mapping
1	[$\frac{2}{3}$, $\frac{1}{3}$, $\frac{1}{4}$]	[1,2,3,4,5,6]
2	[$\frac{2}{3}$, $\frac{1}{3}$, $\frac{3}{4}$]	[7,8,9,10,11,12]

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

No.	position	mapping
1	[0, 0, z]	[1,2,3]
2	[0, 0, $\frac{1}{2} - z$]	[4,5,6]
3	[0, 0, -z]	[7,8,9]
4	[0, 0, $z + \frac{1}{2}$]	[10,11,12]

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

No.	position	mapping
1	$[\frac{1}{3}, \frac{2}{3}, z]$	[1,2,3]
2	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2} - z]$	[4,5,6]
3	$[\frac{1}{3}, \frac{2}{3}, -z]$	[7,8,9]
4	$[\frac{1}{3}, \frac{2}{3}, z + \frac{1}{2}]$	[10,11,12]

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

No.	position	mapping
1	$[\frac{2}{3}, \frac{1}{3}, z]$	[1,2,3]
2	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2} - z]$	[4,5,6]
3	$[\frac{2}{3}, \frac{1}{3}, -z]$	[7,8,9]
4	$[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}]$	[10,11,12]

Table 10: Wyckoff site: 6j, site symmetry: ...2'

No.	position	mapping
1	[x, -x, 0]	[1,9]
2	[x, 2x, 0]	[2,7]
3	[-2x, -x, 0]	[3,8]
4	[-2x, -x, $\frac{1}{2}$]	[4,10]
5	[x, -x, $\frac{1}{2}$]	[5,11]
6	[x, 2x, $\frac{1}{2}$]	[6,12]

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

No.	position	mapping
1	$[x, y, \frac{1}{4}]$	[1,5]
2	$[-y, x - y, \frac{1}{4}]$	[2,6]

continued ...

Table 11

No.	position	mapping
3	$[-x + y, -x, \frac{1}{4}]$	[3,4]
4	$[x, x - y, \frac{3}{4}]$	[7,12]
5	$[-x + y, y, \frac{3}{4}]$	[8,10]
6	$[-y, -x, \frac{3}{4}]$	[9,11]

Table 12: Wyckoff site: 121, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[-y, x - y, z]$	[2]
3	$[-x + y, -x, z]$	[3]
4	$[-x + y, -x, \frac{1}{2} - z]$	[4]
5	$[x, y, \frac{1}{2} - z]$	[5]
6	$[-y, x - y, \frac{1}{2} - z]$	[6]
7	$[x, x - y, -z]$	[7]
8	$[-x + y, y, -z]$	[8]
9	$[-y, -x, -z]$	[9]
10	$[-x + y, y, z + \frac{1}{2}]$	[10]
11	$[-y, -x, z + \frac{1}{2}]$	[11]
12	$[x, x - y, z + \frac{1}{2}]$	[12]