

MSG No. 176.144 $P6_3/m1'$ [Type II, hexagonal]

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

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

Table 2: Wyckoff site: 2b, site symmetry: -3..1'

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

Table 3: Wyckoff site: 2c, site symmetry: -6..1'

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

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

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

Table 5: Wyckoff site: 4e, site symmetry: 3..1'

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

Table 6: Wyckoff site: 4f, site symmetry: 3..1'

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

Table 7: Wyckoff site: 6g, site symmetry: -11'

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

Table 8: Wyckoff site: 6h, site symmetry: m..1'

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

Table 9: Wyckoff site: 12i, site symmetry: 11'

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

continued ...

Table 9

No.	position	mapping
12	$[-y, x - y, \frac{1}{2} - z]$	[12, 24]