

MSG No. 177.150 $P6221'$ [Type II, hexagonal]

Table 1: Wyckoff site: 1a, site symmetry: 6221'

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

Table 2: Wyckoff site: 1b, site symmetry: 6221'

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

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

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

Table 4: Wyckoff site: 2d, site symmetry: 3.21'

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

Table 5: Wyckoff site: 2e, site symmetry: 6..1'

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

Table 6: Wyckoff site: 3f, site symmetry: 2221'

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

Table 7: Wyckoff site: 3g, site symmetry: 2221'

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

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

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

Table 9: Wyckoff site: 6i, site symmetry: 2..1'

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

Table 10: Wyckoff site: 6j, site symmetry: .2.1'

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

Table 11: Wyckoff site: 6k, site symmetry: .2.1'

No.	position	mapping
1	$[x, 0, \frac{1}{2}]$	[1,7,13,19]

continued ...

Table 11

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

Table 12: Wyckoff site: 61, site symmetry: ..21'

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

Table 13: Wyckoff site: 6m, site symmetry: ..21'

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

Table 14: Wyckoff site: 12n, site symmetry: 11'

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

continued ...

Table 14

No.	position	mapping
11	$[-x + y, y, -z]$	[11, 23]
12	$[-y, -x, -z]$	[12, 24]