

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:  $\dots 21'$ 

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:  $\dots 21'$ 

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]