

MSG No. 164.88 $P\bar{3}'m'1$ [Type III, trigonal]

Table 1: Wyckoff site: 1a, site symmetry: $-3'm'$.

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

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

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

Table 3: Wyckoff site: 2c, site symmetry: $3m'$.

No.	position	mapping
1	[0, 0, z]	[1, 2, 3, 10, 11, 12]
2	[0, 0, -z]	[4, 5, 6, 7, 8, 9]

Table 4: Wyckoff site: 2d, site symmetry: $3m'$.

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

Table 5: Wyckoff site: 3e, site symmetry: $.2/m'$.

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

Table 6: Wyckoff site: 3f, site symmetry: $.2/m'$.

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

Table 7: Wyckoff site: $6g$, site symmetry: $.2$.

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

Table 8: Wyckoff site: $6h$, site symmetry: $.2$.

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

Table 9: Wyckoff site: $6i$, site symmetry: $.m'$.

No.	position	mapping
1	$[x, -x, z]$	$[1, 11]$
2	$[x, 2x, z]$	$[2, 12]$
3	$[-2x, -x, z]$	$[3, 10]$
4	$[2x, x, -z]$	$[4, 9]$
5	$[-x, x, -z]$	$[5, 7]$
6	$[-x, -2x, -z]$	$[6, 8]$

Table 10: Wyckoff site: $12j$, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	$[1]$
2	$[-y, x - y, z]$	$[2]$
3	$[-x + y, -x, z]$	$[3]$
4	$[x - y, -y, -z]$	$[4]$
5	$[y, x, -z]$	$[5]$
6	$[-x, -x + y, -z]$	$[6]$
7	$[-x, -y, -z]$	$[7]$
8	$[y, -x + y, -z]$	$[8]$
9	$[x - y, x, -z]$	$[9]$

continued ...

Table 10

No.	position	mapping
10	$[-x + y, y, z]$	[10]
11	$[-y, -x, z]$	[11]
12	$[x, x - y, z]$	[12]