

MSG No. 164.89  $P\bar{3}m'1$  [ Type III, trigonal ]

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

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:  $-3m'$ .

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	$[x, 0, 0]$	$[1, 7]$
2	$[0, x, 0]$	$[2, 8]$
3	$[-x, -x, 0]$	$[3, 9]$
4	$[-x, 0, 0]$	$[4, 10]$
5	$[0, -x, 0]$	$[5, 11]$
6	$[x, x, 0]$	$[6, 12]$

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

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

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	$[-x, x, -z]$	$[4, 8]$
5	$[-x, -2x, -z]$	$[5, 9]$
6	$[2x, x, -z]$	$[6, 7]$

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	$[-x, -y, -z]$	$[4]$
5	$[y, -x + y, -z]$	$[5]$
6	$[x - y, x, -z]$	$[6]$
7	$[x - y, -y, -z]$	$[7]$
8	$[y, x, -z]$	$[8]$
9	$[-x, -x + y, -z]$	$[9]$

*continued ...*

Table 10

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