

MSG No. 215.72  $P\bar{4}'3m'$  [ Type III, cubic ]

Table 1: Wyckoff site: 1a, site symmetry:  $-4'3m'$

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:  $-4'3m'$

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

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

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

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

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

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

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

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

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

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

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

Table 8: Wyckoff site: **12h**, site symmetry:  $2..$ 

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

Table 9: Wyckoff site: **12i**, site symmetry:  $..m'$ 

No.	position	mapping
1	$[x, x, z]$	$[1, 20]$
2	$[x, -x, -z]$	$[2, 17]$
3	$[-x, x, -z]$	$[3, 18]$

*continued ...*

Table 9

No.	position	mapping
4	$[-x, -x, z]$	[4,19]
5	$[z, x, x]$	[5,24]
6	$[x, z, x]$	[6,22]
7	$[-x, z, -x]$	[7,13]
8	$[-z, -x, x]$	[8,15]
9	$[-x, -z, x]$	[9,14]
10	$[z, -x, -x]$	[10,16]
11	$[x, -z, -x]$	[11,21]
12	$[-z, x, -x]$	[12,23]

Table 10: Wyckoff site: 24j, site symmetry: 1

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