

MSG No. 164.90 $P_c\bar{3}m1$ [Type IV, trigonal]

Table 1: Wyckoff site: 2a, site symmetry: -3m.

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

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

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

Table 3: Wyckoff site: 4c, 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]
3	[0, 0, $z + \frac{1}{2}$]	[13,14,15,22,23,24]
4	[0, 0, $\frac{1}{2} - z$]	[16,17,18,19,20,21]

Table 4: Wyckoff site: 4d, 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]
3	[$\frac{1}{3}$, $\frac{2}{3}$, $z + \frac{1}{2}$]	[13,14,15,22,23,24]
4	[$\frac{2}{3}$, $\frac{1}{3}$, $\frac{1}{2} - z$]	[16,17,18,19,20,21]

Table 5: Wyckoff site: 6e, 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]
4	[$\frac{1}{2}$, 0, $\frac{1}{2}$]	[13,16,19,22]
5	[0, $\frac{1}{2}$, $\frac{1}{2}$]	[14,17,20,23]
6	[$\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$]	[15,18,21,24]

Table 6: Wyckoff site: **6f**, site symmetry: $.2'/\bar{m}$.

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

Table 7: Wyckoff site: **12g**, 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]
7	$[x, 0, \frac{1}{2}]$	[13,16]
8	$[0, x, \frac{1}{2}]$	[14,17]
9	$[-x, -x, \frac{1}{2}]$	[15,18]
10	$[-x, 0, \frac{1}{2}]$	[19,22]
11	$[0, -x, \frac{1}{2}]$	[20,23]
12	$[x, x, \frac{1}{2}]$	[21,24]

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

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

Table 9: Wyckoff site: 12i, 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]
7	$[x, -x, z + \frac{1}{2}]$	[13,23]
8	$[x, 2x, z + \frac{1}{2}]$	[14,24]
9	$[-2x, -x, z + \frac{1}{2}]$	[15,22]
10	$[2x, x, \frac{1}{2} - z]$	[16,21]
11	$[-x, x, \frac{1}{2} - z]$	[17,19]
12	$[-x, -2x, \frac{1}{2} - z]$	[18,20]

Table 10: Wyckoff site: 24j, 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]
10	$[-x + y, y, z]$	[10]
11	$[-y, -x, z]$	[11]
12	$[x, x - y, z]$	[12]
13	$[x, y, z + \frac{1}{2}]$	[13]
14	$[-y, x - y, z + \frac{1}{2}]$	[14]
15	$[-x + y, -x, z + \frac{1}{2}]$	[15]
16	$[x - y, -y, \frac{1}{2} - z]$	[16]
17	$[y, x, \frac{1}{2} - z]$	[17]
18	$[-x, -x + y, \frac{1}{2} - z]$	[18]
19	$[-x, -y, \frac{1}{2} - z]$	[19]
20	$[y, -x + y, \frac{1}{2} - z]$	[20]
21	$[x - y, x, \frac{1}{2} - z]$	[21]
22	$[-x + y, y, z + \frac{1}{2}]$	[22]
23	$[-y, -x, z + \frac{1}{2}]$	[23]
24	$[x, x - y, z + \frac{1}{2}]$	[24]