

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

Table 1: Wyckoff site: 2a, site symmetry: $\bar{3}m$.

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: $\bar{3}'m$.

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: $.2'/m$.

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]