

MSG No. 179.166 P_c6_522 [Type IV, hexagonal]

Table 1: Wyckoff site: 6a, site symmetry: 2'2'2

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

Table 2: Wyckoff site: 6b, site symmetry: 2'22'

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

Table 3: Wyckoff site: 6c, site symmetry: 2'2'2

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

Table 4: Wyckoff site: 6d, site symmetry: 2'22'

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

Table 5: Wyckoff site: 12e, site symmetry: 2' . .

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

Table 6: Wyckoff site: 12f, site symmetry: 2' . .

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

Table 7: Wyckoff site: 12g, site symmetry: .2' .

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

continued ...

Table 7

No.	position	mapping
10	$[x, x, \frac{1}{12}]$	[10,14]
11	$[-x, 0, \frac{3}{4}]$	[11,16]
12	$[0, -x, \frac{5}{12}]$	[12,18]

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

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

Table 9: Wyckoff site: 12i, site symmetry: . .2

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

Table 10: Wyckoff site: 12j, site symmetry: ...2'

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

Table 11: Wyckoff site: 24k, site symmetry: 1

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