

MSG No. 175.142 P_c6/m [Type IV, hexagonal]

Table 1: Wyckoff site: 2a, site symmetry: 6/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: 6/m'..

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

Table 3: Wyckoff site: 4c, site symmetry: -6..

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

Table 4: Wyckoff site: 4d, site symmetry: -6'..

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

Table 5: Wyckoff site: 4e, site symmetry: 6..

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

Table 6: Wyckoff site: 6f, site symmetry: 2/m..

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

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

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

Table 8: Wyckoff site: 8h, site symmetry: 3..

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

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

No.	position	mapping
1	$[\frac{1}{2}, 0, z]$	[1,4]
2	$[\frac{1}{2}, \frac{1}{2}, z]$	[2,5]
3	$[0, \frac{1}{2}, z]$	[3,6]
4	$[\frac{1}{2}, 0, -z]$	[7,10]
5	$[\frac{1}{2}, \frac{1}{2}, -z]$	[8,11]
6	$[0, \frac{1}{2}, -z]$	[9,12]
7	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	[13,16]

continued ...

Table 9

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

Table 10: Wyckoff site: 12j, site symmetry: $m\ldots$

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

Table 11: Wyckoff site: 12k, site symmetry: $m'\ldots$

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

Table 12: Wyckoff site: 241, site symmetry: 1

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