

MSG No. 192.244 $P6/mcc1'$ [Type II, hexagonal]

Table 1: Wyckoff site: 2a, site symmetry: 6221'

No.	position	mapping
1	$[0, 0, \frac{1}{4}]$	$[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36]$
2	$[0, 0, \frac{3}{4}]$	$[13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48]$

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

No.	position	mapping
1	$[0, 0, 0]$	$[1, 2, 3, 4, 5, 6, 13, 14, 15, 16, 17, 18, 25, 26, 27, 28, 29, 30, 37, 38, 39, 40, 41, 42]$
2	$[0, 0, \frac{1}{2}]$	$[7, 8, 9, 10, 11, 12, 19, 20, 21, 22, 23, 24, 31, 32, 33, 34, 35, 36, 43, 44, 45, 46, 47, 48]$

Table 3: Wyckoff site: 4c, site symmetry: 3.21'

No.	position	mapping
1	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{4}]$	$[1, 3, 5, 10, 11, 12, 25, 27, 29, 34, 35, 36]$
2	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{4}]$	$[2, 4, 6, 7, 8, 9, 26, 28, 30, 31, 32, 33]$
3	$[\frac{2}{3}, \frac{1}{3}, \frac{3}{4}]$	$[13, 15, 17, 22, 23, 24, 37, 39, 41, 46, 47, 48]$
4	$[\frac{1}{3}, \frac{2}{3}, \frac{3}{4}]$	$[14, 16, 18, 19, 20, 21, 38, 40, 42, 43, 44, 45]$

Table 4: Wyckoff site: 4d, site symmetry: -6..1'

No.	position	mapping
1	$[\frac{1}{3}, \frac{2}{3}, 0]$	$[1, 3, 5, 14, 16, 18, 25, 27, 29, 38, 40, 42]$
2	$[\frac{2}{3}, \frac{1}{3}, 0]$	$[2, 4, 6, 13, 15, 17, 26, 28, 30, 37, 39, 41]$
3	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$	$[7, 8, 9, 22, 23, 24, 31, 32, 33, 46, 47, 48]$
4	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$	$[10, 11, 12, 19, 20, 21, 34, 35, 36, 43, 44, 45]$

Table 5: Wyckoff site: 4e, site symmetry: 6..1'

No.	position	mapping
1	$[0, 0, z]$	$[1, 2, 3, 4, 5, 6, 25, 26, 27, 28, 29, 30]$
2	$[0, 0, \frac{1}{2} - z]$	$[7, 8, 9, 10, 11, 12, 31, 32, 33, 34, 35, 36]$
3	$[0, 0, -z]$	$[13, 14, 15, 16, 17, 18, 37, 38, 39, 40, 41, 42]$
4	$[0, 0, z + \frac{1}{2}]$	$[19, 20, 21, 22, 23, 24, 43, 44, 45, 46, 47, 48]$

Table 6: Wyckoff site: 6f, site symmetry: 2221'

No.	position	mapping
1	$[\frac{1}{2}, 0, \frac{1}{4}]$	[1, 4, 7, 11, 25, 28, 31, 35]
2	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$	[2, 5, 9, 10, 26, 29, 33, 34]
3	$[0, \frac{1}{2}, \frac{1}{4}]$	[3, 6, 8, 12, 27, 30, 32, 36]
4	$[\frac{1}{2}, 0, \frac{3}{4}]$	[13, 16, 19, 23, 37, 40, 43, 47]
5	$[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$	[14, 17, 21, 22, 38, 41, 45, 46]
6	$[0, \frac{1}{2}, \frac{3}{4}]$	[15, 18, 20, 24, 39, 42, 44, 48]

Table 7: Wyckoff site: 6g, site symmetry: 2/m..1'

No.	position	mapping
1	$[\frac{1}{2}, 0, 0]$	[1, 4, 13, 16, 25, 28, 37, 40]
2	$[\frac{1}{2}, \frac{1}{2}, 0]$	[2, 5, 14, 17, 26, 29, 38, 41]
3	$[0, \frac{1}{2}, 0]$	[3, 6, 15, 18, 27, 30, 39, 42]
4	$[\frac{1}{2}, 0, \frac{1}{2}]$	[7, 11, 19, 23, 31, 35, 43, 47]
5	$[0, \frac{1}{2}, \frac{1}{2}]$	[8, 12, 20, 24, 32, 36, 44, 48]
6	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[9, 10, 21, 22, 33, 34, 45, 46]

Table 8: Wyckoff site: 8h, site symmetry: 3..1'

No.	position	mapping
1	$[\frac{1}{3}, \frac{2}{3}, z]$	[1, 3, 5, 25, 27, 29]
2	$[\frac{2}{3}, \frac{1}{3}, z]$	[2, 4, 6, 26, 28, 30]
3	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2} - z]$	[7, 8, 9, 31, 32, 33]
4	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2} - z]$	[10, 11, 12, 34, 35, 36]
5	$[\frac{2}{3}, \frac{1}{3}, -z]$	[13, 15, 17, 37, 39, 41]
6	$[\frac{1}{3}, \frac{2}{3}, -z]$	[14, 16, 18, 38, 40, 42]
7	$[\frac{1}{3}, \frac{2}{3}, z + \frac{1}{2}]$	[19, 20, 21, 43, 44, 45]
8	$[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}]$	[22, 23, 24, 46, 47, 48]

Table 9: Wyckoff site: 12i, site symmetry: 2..1'

No.	position	mapping
1	$[\frac{1}{2}, 0, z]$	[1, 4, 25, 28]
2	$[\frac{1}{2}, \frac{1}{2}, z]$	[2, 5, 26, 29]
3	$[0, \frac{1}{2}, z]$	[3, 6, 27, 30]
4	$[\frac{1}{2}, 0, \frac{1}{2} - z]$	[7, 11, 31, 35]
5	$[0, \frac{1}{2}, \frac{1}{2} - z]$	[8, 12, 32, 36]
6	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	[9, 10, 33, 34]
7	$[\frac{1}{2}, 0, -z]$	[13, 16, 37, 40]

continued ...

Table 9

No.	position	mapping
8	$[\frac{1}{2}, \frac{1}{2}, -z]$	[14,17,38,41]
9	$[0, \frac{1}{2}, -z]$	[15,18,39,42]
10	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	[19,23,43,47]
11	$[0, \frac{1}{2}, z + \frac{1}{2}]$	[20,24,44,48]
12	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[21,22,45,46]

Table 10: Wyckoff site: 12j, site symmetry: .2.1'

No.	position	mapping
1	$[x, 0, \frac{1}{4}]$	[1,7,25,31]
2	$[x, x, \frac{1}{4}]$	[2,10,26,34]
3	$[0, x, \frac{1}{4}]$	[3,8,27,32]
4	$[-x, 0, \frac{1}{4}]$	[4,11,28,35]
5	$[-x, -x, \frac{1}{4}]$	[5,9,29,33]
6	$[0, -x, \frac{1}{4}]$	[6,12,30,36]
7	$[-x, 0, \frac{3}{4}]$	[13,19,37,43]
8	$[-x, -x, \frac{3}{4}]$	[14,22,38,46]
9	$[0, -x, \frac{3}{4}]$	[15,20,39,44]
10	$[x, 0, \frac{3}{4}]$	[16,23,40,47]
11	$[x, x, \frac{3}{4}]$	[17,21,41,45]
12	$[0, x, \frac{3}{4}]$	[18,24,42,48]

Table 11: Wyckoff site: 12k, site symmetry: ..21'

No.	position	mapping
1	$[x, 2x, \frac{1}{4}]$	[1,11,25,35]
2	$[-x, x, \frac{1}{4}]$	[2,9,26,33]
3	$[-2x, -x, \frac{1}{4}]$	[3,12,27,36]
4	$[-x, -2x, \frac{1}{4}]$	[4,7,28,31]
5	$[x, -x, \frac{1}{4}]$	[5,10,29,34]
6	$[2x, x, \frac{1}{4}]$	[6,8,30,32]
7	$[-x, -2x, \frac{3}{4}]$	[13,23,37,47]
8	$[x, -x, \frac{3}{4}]$	[14,21,38,45]
9	$[2x, x, \frac{3}{4}]$	[15,24,39,48]
10	$[x, 2x, \frac{3}{4}]$	[16,19,40,43]
11	$[-x, x, \frac{3}{4}]$	[17,22,41,46]
12	$[-2x, -x, \frac{3}{4}]$	[18,20,42,44]

Table 12: Wyckoff site: 121, site symmetry: $m..1'$

No.	position	mapping
1	$[x, y, 0]$	[1, 16, 25, 40]
2	$[x - y, x, 0]$	[2, 17, 26, 41]
3	$[-y, x - y, 0]$	[3, 18, 27, 42]
4	$[-x, -y, 0]$	[4, 13, 28, 37]
5	$[-x + y, -x, 0]$	[5, 14, 29, 38]
6	$[y, -x + y, 0]$	[6, 15, 30, 39]
7	$[x - y, -y, \frac{1}{2}]$	[7, 23, 31, 47]
8	$[y, x, \frac{1}{2}]$	[8, 24, 32, 48]
9	$[-x, -x + y, \frac{1}{2}]$	[9, 22, 33, 46]
10	$[x, x - y, \frac{1}{2}]$	[10, 21, 34, 45]
11	$[-x + y, y, \frac{1}{2}]$	[11, 19, 35, 43]
12	$[-y, -x, \frac{1}{2}]$	[12, 20, 36, 44]

Table 13: Wyckoff site: 24m, site symmetry: $11'$

No.	position	mapping
1	$[x, y, z]$	[1, 25]
2	$[x - y, x, z]$	[2, 26]
3	$[-y, x - y, z]$	[3, 27]
4	$[-x, -y, z]$	[4, 28]
5	$[-x + y, -x, z]$	[5, 29]
6	$[y, -x + y, z]$	[6, 30]
7	$[x - y, -y, \frac{1}{2} - z]$	[7, 31]
8	$[y, x, \frac{1}{2} - z]$	[8, 32]
9	$[-x, -x + y, \frac{1}{2} - z]$	[9, 33]
10	$[x, x - y, \frac{1}{2} - z]$	[10, 34]
11	$[-x + y, y, \frac{1}{2} - z]$	[11, 35]
12	$[-y, -x, \frac{1}{2} - z]$	[12, 36]
13	$[-x, -y, -z]$	[13, 37]
14	$[-x + y, -x, -z]$	[14, 38]
15	$[y, -x + y, -z]$	[15, 39]
16	$[x, y, -z]$	[16, 40]
17	$[x - y, x, -z]$	[17, 41]
18	$[-y, x - y, -z]$	[18, 42]
19	$[-x + y, y, z + \frac{1}{2}]$	[19, 43]
20	$[-y, -x, z + \frac{1}{2}]$	[20, 44]
21	$[x, x - y, z + \frac{1}{2}]$	[21, 45]
22	$[-x, -x + y, z + \frac{1}{2}]$	[22, 46]
23	$[x - y, -y, z + \frac{1}{2}]$	[23, 47]
24	$[y, x, z + \frac{1}{2}]$	[24, 48]