

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	$[y, x, z + \frac{1}{2}]$	$[24, 48]$