

MPG No. 27.2.101 $6/mmm1'$ [Type II, hexagonal]

Table 1: Wyckoff site: 1o, site symmetry: $6/mmm1'$

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

Table 2: Wyckoff site: 2a, site symmetry: $6mm$

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

Table 3: Wyckoff site: 6b, site symmetry: $m2m$

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

Table 4: Wyckoff site: 6c, site symmetry: $mm2$

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

Table 5: Wyckoff site: 12d, site symmetry: $..m$

No.	position	mapping
1	$[x, 0, z]$	[1, 22, 25, 46]
2	$[0, x, z]$	[3, 24, 27, 48]

continued ...

Table 5

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

Table 6: Wyckoff site: 12e, site symmetry: $\bar{3}m$.

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

Table 7: Wyckoff site: 12f, site symmetry: $m\bar{3}$.

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

Table 8: Wyckoff site: $24g$, site symmetry: 1

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