

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: .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..

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]