

MPG No. 29.2.110 $m\bar{3}1'$ [Type II, cubic]

Table 1: Wyckoff site: 1o, site symmetry: m-31'

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: 6a, site symmetry: 2mm.

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

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

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

Table 4: Wyckoff site: 12c, site symmetry: m..

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

continued ...

Table 4

No.	position	mapping
10	$[-y, z, 0]$	[7, 18, 31, 42]
11	$[y, -z, 0]$	[6, 19, 30, 43]
12	$[-y, -z, 0]$	[8, 17, 32, 41]

Table 5: Wyckoff site: 24d, site symmetry: 1

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