

MPG No. 31.2.116 $\bar{4}3m1'$ [Type II, cubic]

Table 1: Wyckoff site: 1o, site symmetry: $\bar{4}3m1'$

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: 4a, site symmetry: $.3m$

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

Table 3: Wyckoff site: 6b, site symmetry: $2.mm$

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

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

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

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	$[y, x, z]$	$[13, 37]$
14	$[-y, -x, z]$	$[16, 40]$
15	$[y, -x, -z]$	$[14, 38]$
16	$[-y, x, -z]$	$[15, 39]$
17	$[x, z, y]$	$[17, 41]$
18	$[-x, z, -y]$	$[19, 43]$
19	$[-x, -z, y]$	$[20, 44]$
20	$[x, -z, -y]$	$[18, 42]$
21	$[z, y, x]$	$[21, 45]$
22	$[z, -y, -x]$	$[22, 46]$
23	$[-z, y, -x]$	$[23, 47]$
24	$[-z, -y, x]$	$[24, 48]$