

MPG No. 31.3.117  $\bar{4}3m'$  [ Type III, cubic ]

Table 1: Wyckoff site: 1o, site symmetry:  $-4'3m'$

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]

Table 2: Wyckoff site: 4a, site symmetry:  $.3m$

No.	position	mapping
1	[ $x, x, x$ ]	[1,5,9,13,17,21]
2	[ $-x, -x, x$ ]	[4,8,12,16,20,24]
3	[ $-x, x, -x$ ]	[3,7,11,15,19,23]
4	[ $x, -x, -x$ ]	[2,6,10,14,18,22]

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

No.	position	mapping
1	[ $x, 0, 0$ ]	[1,2,17,18]
2	[ $-x, 0, 0$ ]	[3,4,19,20]
3	[0, $x, 0$ ]	[9,11,13,15]
4	[0, $-x, 0$ ]	[10,12,14,16]
5	[0, 0, $x$ ]	[5,8,21,24]
6	[0, 0, $-x$ ]	[6,7,22,23]

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

No.	position	mapping
1	[ $x, x, z$ ]	[1,13]
2	[ $-x, -x, z$ ]	[4,16]
3	[ $-x, x, -z$ ]	[3,15]
4	[ $x, -x, -z$ ]	[2,14]
5	[ $z, x, x$ ]	[9,21]
6	[ $z, -x, -x$ ]	[10,22]
7	[ $-z, -x, x$ ]	[12,24]
8	[ $-z, x, -x$ ]	[11,23]
9	[ $x, z, x$ ]	[5,17]
10	[ $-x, z, -x$ ]	[7,19]
11	[ $x, -z, -x$ ]	[6,18]
12	[ $-x, -z, x$ ]	[8,20]

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

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[-x, -y, z]$	[4]
3	$[-x, y, -z]$	[3]
4	$[x, -y, -z]$	[2]
5	$[z, x, y]$	[9]
6	$[z, -x, -y]$	[10]
7	$[-z, -x, y]$	[12]
8	$[-z, x, -y]$	[11]
9	$[y, z, x]$	[5]
10	$[-y, z, -x]$	[7]
11	$[y, -z, -x]$	[6]
12	$[-y, -z, x]$	[8]
13	$[y, x, z]$	[13]
14	$[-y, -x, z]$	[16]
15	$[y, -x, -z]$	[14]
16	$[-y, x, -z]$	[15]
17	$[x, z, y]$	[17]
18	$[-x, z, -y]$	[19]
19	$[-x, -z, y]$	[20]
20	$[x, -z, -y]$	[18]
21	$[z, y, x]$	[21]
22	$[z, -y, -x]$	[22]
23	$[-z, y, -x]$	[23]
24	$[-z, -y, x]$	[24]