

PG No. 31 $T_d \bar{4}3m$ [cubic]

Table 1: Wyckoff site: 1o, site symmetry: $-43m$

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	[$-x, -x, x$]	[2,7,12,14,19,24]
3	[$-x, x, -x$]	[3,8,10,16,18,23]
4	[$x, -x, -x$]	[4,6,11,15,20,22]

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

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

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

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

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

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