

PG No. 28 T 23 [cubic]

Table 1: Wyckoff site: 1o, site symmetry: 23.

No.	position	mapping
1	[0, 0, 0]	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]

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

No.	position	mapping
1	[x, x, x]	[1, 5, 9]
2	[$-x, -x, x$]	[2, 7, 12]
3	[$-x, x, -x$]	[3, 8, 10]
4	[$x, -x, -x$]	[4, 6, 11]

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

No.	position	mapping
1	[$x, 0, 0$]	[1, 4]
2	[$-x, 0, 0$]	[2, 3]
3	[0, $x, 0$]	[5, 8]
4	[0, $-x, 0$]	[6, 7]
5	[0, 0, x]	[9, 12]
6	[0, 0, $-x$]	[10, 11]

Table 4: Wyckoff site: 12c, 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]