

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]