

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]