

# PG No. 29   $T_h$   $m\bar{3}$   [ cubic ]

Table 1: Wyckoff site: **1o**, site symmetry: **m-3**.

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: **6a**, site symmetry: **2mm**.

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

Table 3: Wyckoff site: **8b**, 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]
5	[-x, -x, -x]	[13,17,21]
6	[x, x, -x]	[14,19,24]
7	[x, -x, x]	[15,20,22]
8	[-x, x, x]	[16,18,23]

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

No.	position	mapping
1	[0, y, z]	[1,16]
2	[0, -y, z]	[2,15]
3	[0, y, -z]	[3,14]
4	[0, -y, -z]	[4,13]
5	[z, 0, y]	[5,20]
6	[z, 0, -y]	[6,19]
7	[-z, 0, y]	[7,18]
8	[-z, 0, -y]	[8,17]
9	[y, z, 0]	[9,24]
10	[-y, z, 0]	[10,23]

*continued ...*

Table 4

No.	position	mapping
11	$[y, -z, 0]$	[11,22]
12	$[-y, -z, 0]$	[12,21]

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	$[-x, -y, -z]$	[13]
14	$[x, y, -z]$	[14]
15	$[x, -y, z]$	[15]
16	$[-x, y, z]$	[16]
17	$[-z, -x, -y]$	[17]
18	$[-z, x, y]$	[18]
19	$[z, x, -y]$	[19]
20	$[z, -x, y]$	[20]
21	$[-y, -z, -x]$	[21]
22	$[y, -z, x]$	[22]
23	$[-y, z, x]$	[23]
24	$[y, z, -x]$	[24]