

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

Table 1: Wyckoff site: 1o, site symmetry: $m\bar{3}$.

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]