

MPG No. 15.2.54 $4/mmm1'$ [Type II, tetragonal]

Table 1: Wyckoff site: 1o, site symmetry: $4/mmm1'$

No.	position	mapping
1	$[0, 0, 0]$	$[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32]$

Table 2: Wyckoff site: 2a, site symmetry: $4mm$

No.	position	mapping
1	$[0, 0, z]$	$[1, 4, 6, 7, 10, 11, 13, 16, 17, 20, 22, 23, 26, 27, 29, 32]$
2	$[0, 0, -z]$	$[2, 3, 5, 8, 9, 12, 14, 15, 18, 19, 21, 24, 25, 28, 30, 31]$

Table 3: Wyckoff site: 4b, site symmetry: $m.m2$

No.	position	mapping
1	$[x, x, 0]$	$[1, 8, 12, 13, 17, 24, 28, 29]$
2	$[-x, -x, 0]$	$[4, 5, 9, 16, 20, 21, 25, 32]$
3	$[-x, x, 0]$	$[3, 6, 10, 15, 19, 22, 26, 31]$
4	$[x, -x, 0]$	$[2, 7, 11, 14, 18, 23, 27, 30]$

Table 4: Wyckoff site: 4c, site symmetry: $m2m.$

No.	position	mapping
1	$[x, 0, 0]$	$[1, 2, 11, 12, 17, 18, 27, 28]$
2	$[-x, 0, 0]$	$[3, 4, 9, 10, 19, 20, 25, 26]$
3	$[0, x, 0]$	$[6, 8, 13, 15, 22, 24, 29, 31]$
4	$[0, -x, 0]$	$[5, 7, 14, 16, 21, 23, 30, 32]$

Table 5: Wyckoff site: 8d, site symmetry: $m.$

No.	position	mapping
1	$[x, y, 0]$	$[1, 12, 17, 28]$
2	$[-x, -y, 0]$	$[4, 9, 20, 25]$
3	$[-y, x, 0]$	$[6, 15, 22, 31]$
4	$[y, -x, 0]$	$[7, 14, 23, 30]$
5	$[-x, y, 0]$	$[3, 10, 19, 26]$
6	$[x, -y, 0]$	$[2, 11, 18, 27]$

continued ...

Table 5

No.	position	mapping
7	$[y, x, 0]$	$[8, 13, 24, 29]$
8	$[-y, -x, 0]$	$[5, 16, 21, 32]$

Table 6: Wyckoff site: **8e**, site symmetry: $\bar{3}m$

No.	position	mapping
1	$[x, x, z]$	$[1, 13, 17, 29]$
2	$[-x, -x, z]$	$[4, 16, 20, 32]$
3	$[-x, x, z]$	$[6, 10, 22, 26]$
4	$[x, -x, z]$	$[7, 11, 23, 27]$
5	$[-x, x, -z]$	$[3, 15, 19, 31]$
6	$[x, -x, -z]$	$[2, 14, 18, 30]$
7	$[x, x, -z]$	$[8, 12, 24, 28]$
8	$[-x, -x, -z]$	$[5, 9, 21, 25]$

Table 7: Wyckoff site: **8f**, site symmetry: $\bar{3}m$

No.	position	mapping
1	$[x, 0, z]$	$[1, 11, 17, 27]$
2	$[-x, 0, z]$	$[4, 10, 20, 26]$
3	$[0, x, z]$	$[6, 13, 22, 29]$
4	$[0, -x, z]$	$[7, 16, 23, 32]$
5	$[-x, 0, -z]$	$[3, 9, 19, 25]$
6	$[x, 0, -z]$	$[2, 12, 18, 28]$
7	$[0, x, -z]$	$[8, 15, 24, 31]$
8	$[0, -x, -z]$	$[5, 14, 21, 30]$

Table 8: Wyckoff site: **16g**, site symmetry: $\bar{3}m$

No.	position	mapping
1	$[x, y, z]$	$[1, 17]$
2	$[-x, -y, z]$	$[4, 20]$
3	$[-y, x, z]$	$[6, 22]$
4	$[y, -x, z]$	$[7, 23]$
5	$[-x, y, -z]$	$[3, 19]$
6	$[x, -y, -z]$	$[2, 18]$
7	$[y, x, -z]$	$[8, 24]$
8	$[-y, -x, -z]$	$[5, 21]$
9	$[-x, -y, -z]$	$[9, 25]$

continued ...

Table 8

No.	position	mapping
10	$[x, y, -z]$	$[12, 28]$
11	$[y, -x, -z]$	$[14, 30]$
12	$[-y, x, -z]$	$[15, 31]$
13	$[x, -y, z]$	$[11, 27]$
14	$[-x, y, z]$	$[10, 26]$
15	$[-y, -x, z]$	$[16, 32]$
16	$[y, x, z]$	$[13, 29]$