

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

No.	position	mapping
1	$[0, 0, 0]$	$[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16]$

Table 2: Wyckoff site: $2a$, site symmetry: $4'm'm$

No.	position	mapping
1	$[0, 0, z]$	$[1, 4, 5, 8, 10, 11, 14, 15]$
2	$[0, 0, -z]$	$[2, 3, 6, 7, 9, 12, 13, 16]$

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

No.	position	mapping
1	$[x, x, 0]$	$[1, 5, 12, 16]$
2	$[-x, -x, 0]$	$[4, 8, 9, 13]$
3	$[-x, x, 0]$	$[3, 7, 10, 14]$
4	$[x, -x, 0]$	$[2, 6, 11, 15]$

Table 4: Wyckoff site: $4c$, site symmetry: $m'2m.$

No.	position	mapping
1	$[x, 0, 0]$	$[1, 2, 15, 16]$
2	$[-x, 0, 0]$	$[3, 4, 13, 14]$
3	$[0, x, 0]$	$[5, 7, 10, 12]$
4	$[0, -x, 0]$	$[6, 8, 9, 11]$

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

No.	position	mapping
1	$[x, y, 0]$	$[1, 16]$
2	$[-x, -y, 0]$	$[4, 13]$
3	$[-y, x, 0]$	$[7, 10]$
4	$[y, -x, 0]$	$[6, 11]$
5	$[-x, y, 0]$	$[3, 14]$
6	$[x, -y, 0]$	$[2, 15]$
7	$[y, x, 0]$	$[5, 12]$

continued ...

Table 5

No.	position	mapping
8	$[-y, -x, 0]$	$[8, 9]$

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

No.	position	mapping
1	$[x, x, z]$	$[1, 5]$
2	$[-x, -x, z]$	$[4, 8]$
3	$[-x, x, z]$	$[10, 14]$
4	$[x, -x, z]$	$[11, 15]$
5	$[-x, x, -z]$	$[3, 7]$
6	$[x, -x, -z]$	$[2, 6]$
7	$[x, x, -z]$	$[12, 16]$
8	$[-x, -x, -z]$	$[9, 13]$

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

No.	position	mapping
1	$[x, 0, z]$	$[1, 15]$
2	$[-x, 0, z]$	$[4, 14]$
3	$[0, x, z]$	$[5, 10]$
4	$[0, -x, z]$	$[8, 11]$
5	$[-x, 0, -z]$	$[3, 13]$
6	$[x, 0, -z]$	$[2, 16]$
7	$[0, x, -z]$	$[7, 12]$
8	$[0, -x, -z]$	$[6, 9]$

Table 8: Wyckoff site: $16g$, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	$[1]$
2	$[-x, -y, z]$	$[4]$
3	$[-y, x, z]$	$[10]$
4	$[y, -x, z]$	$[11]$
5	$[-x, y, -z]$	$[3]$
6	$[x, -y, -z]$	$[2]$
7	$[y, x, -z]$	$[12]$
8	$[-y, -x, -z]$	$[9]$
9	$[-x, -y, -z]$	$[13]$
10	$[x, y, -z]$	$[16]$

continued ...

Table 8

No.	position	mapping
11	$[y, -x, -z]$	[6]
12	$[-y, x, -z]$	[7]
13	$[x, -y, z]$	[15]
14	$[-x, y, z]$	[14]
15	$[-y, -x, z]$	[8]
16	$[y, x, z]$	[5]