

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

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: $4mm$

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

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

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

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

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

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

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

continued ...

Table 5

No.	position	mapping
8	$[-y, -x, 0]$	$[8, 11]$

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

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

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

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

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

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

continued ...

Table 8

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