

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:  $4m'm'$ 

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

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

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

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

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

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

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

*continued ...*

Table 5

No.	position	mapping
8	$[-y, -x, 0]$	$[5, 16]$

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

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

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

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

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

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

*continued ...*

Table 8

No.	position	mapping
11	$[y, -x, -z]$	[14]
12	$[-y, x, -z]$	[15]
13	$[x, -y, z]$	[11]
14	$[-x, y, z]$	[10]
15	$[-y, -x, z]$	[16]
16	$[y, x, z]$	[13]