

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:  $. . m$ 

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:  $. m$ .

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:  $1$ 

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]