

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

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: $4'mm'$

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

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

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

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

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

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

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

continued ...

Table 5

No.	position	mapping
8	$[-y, -x, 0]$	[3,8]

Table 6: Wyckoff site: $8e$, site symmetry: $. . m$

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

Table 7: Wyckoff site: $8f$, site symmetry: $. m$.

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

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

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

continued ...

Table 8

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