

MPG No. 15.6.58 $4/m\bar{m}'m'$ [Type III, tetragonal]

Table 1: Wyckoff site: 1o , site symmetry: $4/\text{mm}'\text{m}'$

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: $4\text{m}'\text{m}'$

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

Table 3: Wyckoff site: 4b , site symmetry: $\text{m}.\text{m}2'$

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

Table 4: Wyckoff site: 4c , site symmetry: $\text{m}2'\text{m}$.

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

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]	[3, 8]
4	[y , $-x$, 0]	[4, 7]
5	[$-x$, y , 0]	[10, 13]
6	[x , $-y$, 0]	[9, 14]
7	[y , x , 0]	[12, 15]

continued ...

Table 5

No.	position	mapping
8	$[-y, -x, 0]$	[11,16]

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

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

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

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

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

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[-x, -y, z]$	[2]
3	$[-y, x, z]$	[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	$[-x, -y, -z]$	[5]
10	$[x, y, -z]$	[6]

continued ...

Table 8

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