

MPG No. 15.5.57  $4'/m'm'm$  ( $4'/m'm'm$  setting) [ Type III, tetragonal ]

Table 1: Wyckoff site:  $1\text{o}$ , 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:  $2\text{a}$ , site symmetry:  $4'm'm$

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

Table 3: Wyckoff site:  $4\text{b}$ , site symmetry:  $m'.m2'$

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

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

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

Table 5: Wyckoff site:  $8\text{d}$ , site symmetry:  $m'..$

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

*continued ...*

Table 5

No.	position	mapping
8	$[-y, -x, 0]$	[8,9]

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

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

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

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

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

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

*continued ...*

Table 8

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