

PG No. 15  $D_{4h}$   $4/mmm$  [ tetragonal ]

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:  $4mm$

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:  $m.m2$

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

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

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

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

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

*continued ...*

Table 5

No.	position	mapping
8	$[-y, -x, 0]$	$[8, 15]$

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

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

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

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

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

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

*continued ...*

Table 8

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