

MSG No. 83.43  $P4/m$  [ Type I, tetragonal ]

Table 1: Wyckoff site: 1a, site symmetry:  $4/m..$

No.	position	mapping
1	$[0, 0, 0]$	$[1, 2, 3, 4, 5, 6, 7, 8]$

Table 2: Wyckoff site: 1b, site symmetry:  $4/m..$

No.	position	mapping
1	$[0, 0, \frac{1}{2}]$	$[1, 2, 3, 4, 5, 6, 7, 8]$

Table 3: Wyckoff site: 1c, site symmetry:  $4/m..$

No.	position	mapping
1	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[1, 2, 3, 4, 5, 6, 7, 8]$

Table 4: Wyckoff site: 1d, site symmetry:  $4/m..$

No.	position	mapping
1	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[1, 2, 3, 4, 5, 6, 7, 8]$

Table 5: Wyckoff site: 2e, site symmetry:  $2/m..$

No.	position	mapping
1	$[0, \frac{1}{2}, 0]$	$[1, 4, 5, 8]$
2	$[\frac{1}{2}, 0, 0]$	$[2, 3, 6, 7]$

Table 6: Wyckoff site: 2f, site symmetry:  $2/m..$

No.	position	mapping
1	$[0, \frac{1}{2}, \frac{1}{2}]$	$[1, 4, 5, 8]$
2	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[2, 3, 6, 7]$

Table 7: Wyckoff site: 2g, site symmetry: 4 . .

No.	position	mapping
1	$[0, 0, z]$	$[1, 2, 3, 4]$
2	$[0, 0, -z]$	$[5, 6, 7, 8]$

Table 8: Wyckoff site: 2h, site symmetry: 4 . .

No.	position	mapping
1	$[\frac{1}{2}, \frac{1}{2}, z]$	$[1, 2, 3, 4]$
2	$[\frac{1}{2}, \frac{1}{2}, -z]$	$[5, 6, 7, 8]$

Table 9: Wyckoff site: 4i, site symmetry: 2 . .

No.	position	mapping
1	$[0, \frac{1}{2}, z]$	$[1, 4]$
2	$[\frac{1}{2}, 0, z]$	$[2, 3]$
3	$[0, \frac{1}{2}, -z]$	$[5, 8]$
4	$[\frac{1}{2}, 0, -z]$	$[6, 7]$

Table 10: Wyckoff site: 4j, site symmetry: m . .

No.	position	mapping
1	$[x, y, 0]$	$[1, 8]$
2	$[-y, x, 0]$	$[2, 7]$
3	$[y, -x, 0]$	$[3, 6]$
4	$[-x, -y, 0]$	$[4, 5]$

Table 11: Wyckoff site: 4k, site symmetry: m . .

No.	position	mapping
1	$[x, y, \frac{1}{2}]$	$[1, 8]$
2	$[-y, x, \frac{1}{2}]$	$[2, 7]$
3	$[y, -x, \frac{1}{2}]$	$[3, 6]$
4	$[-x, -y, \frac{1}{2}]$	$[4, 5]$

Table 12: Wyckoff site:  $81$ , site symmetry:  $1$ 

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