

MSG No. 83.44 $P4/m1'$ [Type II, tetragonal]

Table 1: Wyckoff site: 1a, site symmetry: $4/m\ldots 1'$

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: 1b, site symmetry: $4/m\ldots 1'$

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

Table 3: Wyckoff site: 1c, site symmetry: $4/m\ldots 1'$

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

Table 4: Wyckoff site: 1d, site symmetry: $4/m\ldots 1'$

No.	position	mapping
1	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16]$

Table 5: Wyckoff site: 2e, site symmetry: $2/m\ldots 1'$

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

Table 6: Wyckoff site: 2f, site symmetry: $2/m\ldots 1'$

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

Table 7: Wyckoff site: 2g, site symmetry: 4..1'

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

Table 8: Wyckoff site: 2h, site symmetry: 4..1'

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

Table 9: Wyckoff site: 4i, site symmetry: 2..1'

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

Table 10: Wyckoff site: 4j, site symmetry: m..1'

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

Table 11: Wyckoff site: 4k, site symmetry: m..1'

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

Table 12: Wyckoff site: 81, site symmetry: 11'

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