

MSG No. 111.252 $P\bar{4}2m1'$ [Type II, tetragonal]

Table 1: Wyckoff site: 1a, site symmetry: -42m1'

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: -42m1'

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 3: Wyckoff site: 1c, site symmetry: -42m1'

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 4: Wyckoff site: 1d, site symmetry: -42m1'

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 5: Wyckoff site: 2e, site symmetry: 222.1'

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

Table 6: Wyckoff site: 2f, site symmetry: 222.1'

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

Table 7: Wyckoff site: 2g, site symmetry: 2.mmm'

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

Table 8: Wyckoff site: 2h, site symmetry: 2.mmm'

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

Table 9: Wyckoff site: 4i, site symmetry: .2.1'

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

Table 10: Wyckoff site: 4j, site symmetry: .2.1'

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

Table 11: Wyckoff site: 4k, site symmetry: .2.1'

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

Table 12: Wyckoff site: 4l, site symmetry: .2.1'

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

Table 13: Wyckoff site: 4m, site symmetry: 2..1'

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

Table 14: Wyckoff site: 4n, site symmetry: ..m1'

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

Table 15: Wyckoff site: 8o, site symmetry: 11'

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