

MSG No. 111.253 $P\bar{4}'2'm$ [Type III, tetragonal]

Table 1: Wyckoff site: 1a, site symmetry: $-4'2'm$

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

Table 2: Wyckoff site: 1b, site symmetry: $-4'2'm$

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

Table 3: Wyckoff site: 1c, site symmetry: $-4'2'm$

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

Table 4: Wyckoff site: 1d, site symmetry: $-4'2'm$

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

Table 5: Wyckoff site: 2e, site symmetry: $22'2'$.

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

Table 6: Wyckoff site: 2f, site symmetry: $22'2'$.

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

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

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: 2.m̄m

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	[x, 0, 0]	[1,5]
2	[-x, 0, 0]	[2,6]
3	[0, -x, 0]	[3,7]
4	[0, x, 0]	[4,8]

Table 10: Wyckoff site: 4j, site symmetry: .2'.

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

Table 11: Wyckoff site: 4k, site symmetry: .2'.

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

Table 12: Wyckoff site: 41, site symmetry: .2'.

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

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

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

Table 14: Wyckoff site: 4n, site symmetry: ...m

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

Table 15: Wyckoff site: 8o, site symmetry: 1

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]