

MSG No. 111.255 $P\bar{4}2'm'$ [Type III, tetragonal]

Table 1: Wyckoff site: 1a, site symmetry: $-42'm'$

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

Table 2: Wyckoff site: 1b, site symmetry: $-42'm'$

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: $-42'm'$

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

Table 4: Wyckoff site: 1d, site symmetry: $-42'm'$

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: $2.m'm'$

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

Table 8: Wyckoff site: 2h, site symmetry: $2.m'm'$

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

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: $4\mathbf{1}$, 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: $4\mathbf{m}$, 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: $4\mathbf{n}$, site symmetry: $..m'$

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

Table 15: Wyckoff site: $8\mathbf{o}$, 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]