

MSG No. 89.90 $P42'2'$ [Type III, tetragonal]

Table 1: Wyckoff site: 1a, site symmetry: $42'2'$

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

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

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

Table 3: Wyckoff site: 1c, site symmetry: $42'2'$

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: $42'2'$

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: $22'2'$.

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

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

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

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]	[5,6]
4	[\frac{1}{2}, 0, -z]	[7,8]

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

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

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

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

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

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

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

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

Table 14: Wyckoff site: 4n, site symmetry: .2'.

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

Table 15: Wyckoff site: 4o, site symmetry: .2'.

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

Table 16: Wyckoff site: 8p, 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]

continued ...

Table 16

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