

MSG No. 47.250 $Pmmm1'$ [Type II, orthorhombic]

Table 1: Wyckoff site: $1a$, site symmetry: $mmm1'$

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: $mmm1'$

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

Table 3: Wyckoff site: $1c$, site symmetry: $mmm1'$

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: $mmm1'$

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

Table 5: Wyckoff site: $1e$, site symmetry: $mmm1'$

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

Table 6: Wyckoff site: $1f$, site symmetry: $mmm1'$

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 7: Wyckoff site: $1g$, site symmetry: $mmm1'$

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

Table 8: Wyckoff site: $1h$, site symmetry: $mmm1'$

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 9: Wyckoff site: $2i$, site symmetry: $2mm1'$

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

Table 10: Wyckoff site: $2j$, site symmetry: $2mm1'$

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

Table 11: Wyckoff site: $2k$, site symmetry: $2mm1'$

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

Table 12: Wyckoff site: $2l$, site symmetry: $2mm1'$

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

Table 13: Wyckoff site: $2\mathbf{m}$, site symmetry: $\mathbf{m}2\mathbf{m}1'$

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

Table 14: Wyckoff site: $2\mathbf{n}$, site symmetry: $\mathbf{m}2\mathbf{m}1'$

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

Table 15: Wyckoff site: $2\mathbf{o}$, site symmetry: $\mathbf{m}2\mathbf{m}1'$

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

Table 16: Wyckoff site: $2\mathbf{p}$, site symmetry: $\mathbf{m}2\mathbf{m}1'$

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

Table 17: Wyckoff site: $2\mathbf{q}$, site symmetry: $\mathbf{mm}21'$

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

Table 18: Wyckoff site: $2\mathbf{r}$, site symmetry: $\mathbf{mm}21'$

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

Table 19: Wyckoff site: 2s, site symmetry: $\text{mm}21'$

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

Table 20: Wyckoff site: 2t, site symmetry: $\text{mm}21'$

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

Table 21: Wyckoff site: 4u, site symmetry: $\text{m}..1'$

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

Table 22: Wyckoff site: 4v, site symmetry: $\text{m}..1'$

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

Table 23: Wyckoff site: 4w, site symmetry: $..m.1'$

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

Table 24: Wyckoff site: 4x, site symmetry: $\cdot m \cdot 1'$

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

Table 25: Wyckoff site: 4y, site symmetry: $\cdot \cdot m 1'$

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

Table 26: Wyckoff site: 4z, site symmetry: $\cdot \cdot m 1'$

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

Table 27: Wyckoff site: 8A, 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	$[-x, -y, -z]$	$[5, 13]$
6	$[-x, y, z]$	$[6, 14]$
7	$[x, -y, z]$	$[7, 15]$
8	$[x, y, -z]$	$[8, 16]$