

MSG No. 47.255 P_Cmmm [Type IV, orthorhombic]

Table 1: Wyckoff site: 2a, site symmetry: mmm

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

Table 2: Wyckoff site: 2b, site symmetry: mmm

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

Table 3: Wyckoff site: 2c, site symmetry: mmm

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

Table 4: Wyckoff site: 2d, site symmetry: mmm

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

Table 5: Wyckoff site: 4e, site symmetry: $. . 2' / m$

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

Table 6: Wyckoff site: **4f**, site symmetry: $\dots 2'/m$

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

Table 7: Wyckoff site: **4g**, site symmetry: $2mm$

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

Table 8: Wyckoff site: **4h**, site symmetry: $2mm$

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

Table 9: Wyckoff site: **4i**, site symmetry: $m2m$

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

Table 10: Wyckoff site: **4j**, site symmetry: $m2m$

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

Table 11: Wyckoff site: $4k$, site symmetry: $mm2$

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

Table 12: Wyckoff site: $4l$, site symmetry: $mm2$

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

Table 13: Wyckoff site: $8m$, site symmetry: $. . 2'$

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

Table 14: Wyckoff site: $8n$, site symmetry: $m. .$

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

Table 15: Wyckoff site: $8\mathbf{o}$, site symmetry: $\bar{3}m$.

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

Table 16: Wyckoff site: $8\mathbf{p}$, site symmetry: $\bar{3}m$.

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

Table 17: Wyckoff site: $8\mathbf{q}$, site symmetry: $\bar{3}m$.

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

Table 18: Wyckoff site: $16\mathbf{r}$, site symmetry: $\bar{3}m$.

No.	position	mapping
1	$[x, y, z]$	$[1]$
2	$[x, -y, -z]$	$[2]$
3	$[-x, y, -z]$	$[3]$

continued ...

Table 18

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