

SG No. 65  $D_{2h}^{19}$   $Cmmm$  [ orthorhombic ]

\* plus set:  $+ [0, 0, 0], \quad + [\frac{1}{2}, \frac{1}{2}, 0]$

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: 4e, site symmetry:  $\dots 2/m$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Table 13: Wyckoff site:  $8\mathbf{m}$ , site symmetry:  $\bar{3}2$ 

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

Table 14: Wyckoff site:  $8\mathbf{n}$ , site symmetry:  $\mathbf{m}\bar{3}$ 

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

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

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

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

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

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

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

Table 18: Wyckoff site:  $16\mathbf{r}$ , site symmetry:  $1$ 

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