

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

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

Table 1: Wyckoff site: 2a, site symmetry:  $\text{mmm}$

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

Table 2: Wyckoff site: 2b, site symmetry:  $\text{mmm}$

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

Table 3: Wyckoff site: 2c, site symmetry:  $\text{mmm}$

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:  $\text{mmm}$

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

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

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:  $\dots 2/\text{m}$

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: 8m, site symmetry: . . 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: 8n, site symmetry: m..

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: 8o, site symmetry: .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: 8p, site symmetry: . . 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: 8q, site symmetry: . . 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: **16r**, 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]