

SG No. 47 D_{2h}^1 $Pmmm$ [orthorhombic]

* plus set: + [0, 0, 0]

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

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

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

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

Table 3: Wyckoff site: 1c, site symmetry: mmm

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

Table 4: Wyckoff site: 1d, site symmetry: mmm

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

Table 5: Wyckoff site: 1e, site symmetry: mmm

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

Table 6: Wyckoff site: 1f, site symmetry: mmm

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

Table 7: Wyckoff site: 1g, site symmetry: mmm

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

Table 8: Wyckoff site: 1h, site symmetry: mmm

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

Table 9: Wyckoff site: 2i, site symmetry: $2mm$

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

Table 10: Wyckoff site: 2j, 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 11: Wyckoff site: 2k, site symmetry: $2mm$

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

Table 12: Wyckoff site: 2l, site symmetry: $2mm$

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

Table 13: Wyckoff site: $2m$, site symmetry: $m2m$

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

Table 14: Wyckoff site: $2n$, 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 15: Wyckoff site: $2o$, site symmetry: $m2m$

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

Table 16: Wyckoff site: $2p$, site symmetry: $m2m$

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

Table 17: Wyckoff site: $2q$, site symmetry: $mm2$

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

Table 18: Wyckoff site: $2r$, 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 19: Wyckoff site: $2s$, site symmetry: $mm2$

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

Table 20: Wyckoff site: $2t$, site symmetry: $mm2$

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

Table 21: Wyckoff site: $4u$, 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 22: Wyckoff site: $4v$, site symmetry: $m..$

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

Table 23: Wyckoff site: $4w$, 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 24: Wyckoff site: $4x$, site symmetry: $.m$.

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

Table 25: Wyckoff site: $4y$, 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 26: Wyckoff site: $4z$, 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 27: Wyckoff site: $8A$, 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]