

SG No. 49 D_{2h}^3 $Pccm$ [orthorhombic]

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

Table 1: Wyckoff site: **2a**, site symmetry: $\dots 2/m$

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

Table 2: Wyckoff site: **2b**, site symmetry: $\dots 2/m$

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

Table 3: Wyckoff site: **2c**, site symmetry: $\dots 2/m$

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

Table 4: Wyckoff site: **2d**, site symmetry: $\dots 2/m$

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

Table 5: Wyckoff site: **2e**, site symmetry: 222

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

Table 6: Wyckoff site: $2f$, site symmetry: 222

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

Table 7: Wyckoff site: $2g$, site symmetry: 222

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

Table 8: Wyckoff site: $2h$, site symmetry: 222

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

Table 9: Wyckoff site: $4i$, site symmetry: $2..$

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

Table 10: Wyckoff site: $4j$, site symmetry: $2..$

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

Table 11: Wyckoff site: $4\mathbf{k}$, site symmetry: $.2$.

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

Table 12: Wyckoff site: $4\mathbf{l}$, site symmetry: $.2$.

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

Table 13: Wyckoff site: $4\mathbf{m}$, site symmetry: $.2$

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

Table 14: Wyckoff site: $4\mathbf{n}$, site symmetry: $.2$

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

Table 15: Wyckoff site: $4\mathbf{o}$, site symmetry: $.2$

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

Table 16: Wyckoff site: $4\mathbf{p}$, site symmetry: $\dots 2$

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

Table 17: Wyckoff site: $4\mathbf{q}$, site symmetry: $\dots m$

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

Table 18: Wyckoff site: $8\mathbf{r}$, site symmetry: 1

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