# SG No. 118 $D_{2d}^{8}$ $P\bar{4}n2$ [ tetragonal ]

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

Table 1: Wyckoff site: `2a`, site symmetry: `-4..`

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

Table 2: Wyckoff site: `2b`, site symmetry: `-4..`

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

Table 3: Wyckoff site: `2c`, site symmetry: `2.22`

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

Table 4: Wyckoff site: `2d`, site symmetry: `2.22`

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

Table 5: Wyckoff site: `4e`, site symmetry: `2..`

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

Table 6: Wyckoff site: `4f`, site symmetry: `..2`

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

Table 7: Wyckoff site: `4g`, site symmetry: `..2`

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

Table 8: Wyckoff site: `4h`, site symmetry: `2..`

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

Table 9: Wyckoff site: `8i`, site symmetry: `1`

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