# MSG No. 50.281 $Pb'a'n$ [ Type III, orthorhombic ]

Table 1: Wyckoff site: `2a`, site symmetry: `2'2'2`

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

Table 2: Wyckoff site: `2b`, site symmetry: `2'2'2`

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

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

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

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

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

Table 5: Wyckoff site: `4e`, site symmetry: `-1`

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

Table 6: Wyckoff site: `4f`, site symmetry: `-1`

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

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

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

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

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

Table 9: Wyckoff site: `4i`, site symmetry: `.2'.`

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

Table 10: Wyckoff site: `4j`, site symmetry: `.2'.`

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

Table 11: Wyckoff site: `4k`, site symmetry: `..2`

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

Table 12: Wyckoff site: `4l`, site symmetry: `..2`

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

Table 13: Wyckoff site: `8m`, site symmetry: `1`

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