

SG No. 96 D_4^8 $P4_32_12$ [tetragonal]

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

* Wyckoff site: **4a**, site symmetry: $\dots 2$

Table 1: Wyckoff bond: **4a@4a**

| No. | vector | center | mapping |
|-----|---------------|---|-----------|
| 1 | $[X, -X, Z]$ | $[x, x, 0]$ | $[1, -7]$ |
| 2 | $[-X, X, Z]$ | $[-x, -x, \frac{1}{2}]$ | $[2, -8]$ |
| 3 | $[X, X, Z]$ | $[\frac{1}{2} - x, x + \frac{1}{2}, \frac{3}{4}]$ | $[3, -5]$ |
| 4 | $[-X, -X, Z]$ | $[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{4}]$ | $[4, -6]$ |

Table 2: Wyckoff bond: **4b@4a**

| No. | vector | center | mapping |
|-----|---------------|---|----------|
| 1 | $[X, X, 0]$ | $[x, x, 0]$ | $[1, 7]$ |
| 2 | $[-X, -X, 0]$ | $[-x, -x, \frac{1}{2}]$ | $[2, 8]$ |
| 3 | $[-X, X, 0]$ | $[\frac{1}{2} - x, x + \frac{1}{2}, \frac{3}{4}]$ | $[3, 5]$ |
| 4 | $[X, -X, 0]$ | $[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{4}]$ | $[4, 6]$ |

Table 3: Wyckoff bond: **8c@4a**

| No. | vector | center | mapping |
|-----|----------------|---|---------|
| 1 | $[X, Y, Z]$ | $[x, x, 0]$ | $[1]$ |
| 2 | $[-X, -Y, Z]$ | $[-x, -x, \frac{1}{2}]$ | $[2]$ |
| 3 | $[-Y, X, Z]$ | $[\frac{1}{2} - x, x + \frac{1}{2}, \frac{3}{4}]$ | $[3]$ |
| 4 | $[Y, -X, Z]$ | $[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{4}]$ | $[4]$ |
| 5 | $[-X, Y, -Z]$ | $[\frac{1}{2} - x, x + \frac{1}{2}, \frac{3}{4}]$ | $[5]$ |
| 6 | $[X, -Y, -Z]$ | $[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{4}]$ | $[6]$ |
| 7 | $[Y, X, -Z]$ | $[x, x, 0]$ | $[7]$ |
| 8 | $[-Y, -X, -Z]$ | $[-x, -x, \frac{1}{2}]$ | $[8]$ |

* Wyckoff site: **8b**, site symmetry: 1

Table 4: Wyckoff bond: **8a@8b**

| No. | vector | center | mapping |
|-----|---------------|---|---------|
| 1 | $[X, Y, Z]$ | $[x, y, z]$ | $[1]$ |
| 2 | $[-X, -Y, Z]$ | $[-x, -y, z + \frac{1}{2}]$ | $[2]$ |
| 3 | $[-Y, X, Z]$ | $[\frac{1}{2} - y, x + \frac{1}{2}, z + \frac{3}{4}]$ | $[3]$ |
| 4 | $[Y, -X, Z]$ | $[y + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{4}]$ | $[4]$ |
| 5 | $[-X, Y, -Z]$ | $[\frac{1}{2} - x, y + \frac{1}{2}, \frac{3}{4} - z]$ | $[5]$ |

continued ...

Table 4

| No. | vector | center | mapping |
|-----|----------------|---|---------|
| 6 | $[X, -Y, -Z]$ | $[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{4} - z]$ | [6] |
| 7 | $[Y, X, -Z]$ | $[y, x, -z]$ | [7] |
| 8 | $[-Y, -X, -Z]$ | $[-y, -x, \frac{1}{2} - z]$ | [8] |