# SG No. 105 $C_{4v}^{7}$ $P4_2mc$ [ tetragonal ]

* plus set: $+[0,\ 0,\ 0]$
* Wyckoff site: `2a`, site symmetry: `2mm`.

Table 1: Wyckoff bond: `2a@2a`

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

Table 2: Wyckoff bond: `2b@2a`

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

Table 3: Wyckoff bond: `4c@2a`

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

Table 4: Wyckoff bond: `4d@2a`

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

Table 5: Wyckoff bond: `8e@2a`

| No. | vector | center | mapping |
|---|---|---|---|
| 1 | $[X,\ Y,\ Z]$ | $[0,\ 0,\ z]$ | `[1]` |
| 2 | $[-X,\ -Y,\ Z]$ | $[0,\ 0,\ z]$ | `[2]` |
| 3 | $[-Y,\ X,\ Z]$ | $\left[0,\ 0,\ z+\frac{1}{2}\right]$ | `[3]` |
| 4 | $[Y,\ -X,\ Z]$ | $\left[0,\ 0,\ z+\frac{1}{2}\right]$ | `[4]` |

*continued ...*

Table 5

| No. | vector | center | mapping |
|---|---|---|---|
| 5 | $[X, -Y, Z]$ | $[0, 0, z]$ | `[5]` |
| 6 | $[-X, Y, Z]$ | $[0, 0, z]$ | `[6]` |
| 7 | $[-Y, -X, Z]$ | $\left[0, 0, z+\frac{1}{2}\right]$ | `[7]` |
| 8 | $[Y, X, Z]$ | $\left[0, 0, z+\frac{1}{2}\right]$ | `[8]` |

* Wyckoff site: `2b`, site symmetry: `2mm`.

Table 6: Wyckoff bond: `2a@2b`

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

Table 7: Wyckoff bond: `2b@2b`

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

Table 8: Wyckoff bond: `4c@2b`

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

Table 9: Wyckoff bond: `4d@2b`

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

Table 10: Wyckoff bond: `8e@2b`

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

* Wyckoff site: `2c`, site symmetry: `2mm`.

Table 11: Wyckoff bond: `2a@2c`

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

Table 12: Wyckoff bond: `2b@2c`

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

Table 13: Wyckoff bond: `2c@2c`

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

Table 14: Wyckoff bond: `4d@2c`

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

Table 15: Wyckoff bond: `4e@2c`

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

Table 16: Wyckoff bond: `4f@2c`

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

Table 17: Wyckoff bond: `8g@2c`

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

* Wyckoff site: `4d`, site symmetry: `.m.`

Table 18: Wyckoff bond: `4a@4d`

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

Table 19: Wyckoff bond: `4b@4d`

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

Table 20: Wyckoff bond: `8c@4d`

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

* Wyckoff site: `4e`, site symmetry: `.m.`

Table 21: Wyckoff bond: `4a@4e`

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

Table 22: Wyckoff bond: `4b@4e`

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

Table 23: Wyckoff bond: `8c@4e`

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

* Wyckoff site: `8f`, site symmetry: `1`

Table 24: Wyckoff bond: `8a@8f`

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