# SG No. 204 $T_{\mathrm{h}}^{5}$ $Im\bar{3}$ [ cubic ]

* plus set: $+[0,\ 0,\ 0]$, $+\left[\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}\right]$

Table 1: Wyckoff site: `2a`, site symmetry: `m-3.`

| No. | position | mapping |
|---|---|---|
| 1 | $[0,\ 0,\ 0]$ | `[1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24]` |

Table 2: Wyckoff site: `6b`, site symmetry: `mmm..`

| No. | position | mapping |
|---|---|---|
| 1 | $\left[0,\ \frac{1}{2},\ \frac{1}{2}\right]$ | `[1,2,3,4,13,14,15,16]` |
| 2 | $\left[\frac{1}{2},\ 0,\ \frac{1}{2}\right]$ | `[5,6,7,8,17,18,19,20]` |
| 3 | $\left[\frac{1}{2},\ \frac{1}{2},\ 0\right]$ | `[9,10,11,12,21,22,23,24]` |

Table 3: Wyckoff site: `8c`, site symmetry: `.-3.`

| No. | position | mapping |
|---|---|---|
| 1 | $\left[\frac{1}{4},\ \frac{1}{4},\ \frac{1}{4}\right]$ | `[1,5,9,13,17,21]` |
| 2 | $\left[\frac{3}{4},\ \frac{3}{4},\ \frac{1}{4}\right]$ | `[2,7,12,14,19,24]` |
| 3 | $\left[\frac{3}{4},\ \frac{1}{4},\ \frac{3}{4}\right]$ | `[3,8,10,15,20,22]` |
| 4 | $\left[\frac{1}{4},\ \frac{3}{4},\ \frac{3}{4}\right]$ | `[4,6,11,16,18,23]` |

Table 4: Wyckoff site: `12d`, site symmetry: `mm2..`

| No. | position | mapping |
|---|---|---|
| 1 | $[x,\ 0,\ 0]$ | `[1,4,14,15]` |
| 2 | $[-x,\ 0,\ 0]$ | `[2,3,13,16]` |
| 3 | $[0,\ x,\ 0]$ | `[5,8,18,19]` |
| 4 | $[0,\ -x,\ 0]$ | `[6,7,17,20]` |
| 5 | $[0,\ 0,\ x]$ | `[9,12,22,23]` |
| 6 | $[0,\ 0,\ -x]$ | `[10,11,21,24]` |

Table 5: Wyckoff site: `12e`, site symmetry: `mm2..`

| No. | position | mapping |
|---|---|---|
| 1 | $\left[x,\ 0,\ \frac{1}{2}\right]$ | `[1,4,14,15]` |
| 2 | $\left[-x,\ 0,\ \frac{1}{2}\right]$ | `[2,3,13,16]` |
| 3 | $\left[\frac{1}{2},\ x,\ 0\right]$ | `[5,8,18,19]` |

*continued ...*

Table 5

| No. | position | mapping |
|---|---|---|
| 4 | $\left[\frac{1}{2}, -x, 0\right]$ | `[6,7,17,20]` |
| 5 | $\left[0, \frac{1}{2}, x\right]$ | `[9,12,22,23]` |
| 6 | $\left[0, \frac{1}{2}, -x\right]$ | `[10,11,21,24]` |

Table 6: Wyckoff site: `16f`, site symmetry: `.3.`

| No. | position | mapping |
|---|---|---|
| 1 | $[x, x, x]$ | `[1,5,9]` |
| 2 | $[-x, -x, x]$ | `[2,7,12]` |
| 3 | $[-x, x, -x]$ | `[3,8,10]` |
| 4 | $[x, -x, -x]$ | `[4,6,11]` |
| 5 | $[-x, -x, -x]$ | `[13,17,21]` |
| 6 | $[x, x, -x]$ | `[14,19,24]` |
| 7 | $[x, -x, x]$ | `[15,20,22]` |
| 8 | $[-x, x, x]$ | `[16,18,23]` |

Table 7: Wyckoff site: `24g`, site symmetry: `m..`

| No. | position | mapping |
|---|---|---|
| 1 | $[0, y, z]$ | `[1,16]` |
| 2 | $[0, -y, z]$ | `[2,15]` |
| 3 | $[0, y, -z]$ | `[3,14]` |
| 4 | $[0, -y, -z]$ | `[4,13]` |
| 5 | $[z, 0, y]$ | `[5,20]` |
| 6 | $[z, 0, -y]$ | `[6,19]` |
| 7 | $[-z, 0, y]$ | `[7,18]` |
| 8 | $[-z, 0, -y]$ | `[8,17]` |
| 9 | $[y, z, 0]$ | `[9,24]` |
| 10 | $[-y, z, 0]$ | `[10,23]` |
| 11 | $[y, -z, 0]$ | `[11,22]` |
| 12 | $[-y, -z, 0]$ | `[12,21]` |

Table 8: Wyckoff site: `48h`, site symmetry: `1`

| No. | position | mapping |
|---|---|---|
| 1 | $[x, y, z]$ | `[1]` |
| 2 | $[-x, -y, z]$ | `[2]` |
| 3 | $[-x, y, -z]$ | `[3]` |
| 4 | $[x, -y, -z]$ | `[4]` |

*continued ...*

Table 8

| No. | position | mapping |
|---|---|---|
| 5 | $[z, x, y]$ | [5] |
| 6 | $[z, -x, -y]$ | [6] |
| 7 | $[-z, -x, y]$ | [7] |
| 8 | $[-z, x, -y]$ | [8] |
| 9 | $[y, z, x]$ | [9] |
| 10 | $[-y, z, -x]$ | [10] |
| 11 | $[y, -z, -x]$ | [11] |
| 12 | $[-y, -z, x]$ | [12] |
| 13 | $[-x, -y, -z]$ | [13] |
| 14 | $[x, y, -z]$ | [14] |
| 15 | $[x, -y, z]$ | [15] |
| 16 | $[-x, y, z]$ | [16] |
| 17 | $[-z, -x, -y]$ | [17] |
| 18 | $[-z, x, y]$ | [18] |
| 19 | $[z, x, -y]$ | [19] |
| 20 | $[z, -x, y]$ | [20] |
| 21 | $[-y, -z, -x]$ | [21] |
| 22 | $[y, -z, x]$ | [22] |
| 23 | $[-y, z, x]$ | [23] |
| 24 | $[y, z, -x]$ | [24] |