# MSG No. 215.71 $P\bar{4}3m1'$ [ Type II, cubic ]

Table 1: Wyckoff site: `1a`, site symmetry: `-43m1'`

| 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, |
| | | 25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,48] |

Table 2: Wyckoff site: `1b`, site symmetry: `-43m1'`

| No. | position | mapping |
|---|---|---|
| 1 | $\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$ | [1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24, |
| | | 25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,48] |

Table 3: Wyckoff site: `3c`, site symmetry: `-42.m1'`

| No. | position | mapping |
|---|---|---|
| 1 | $\left[0, \frac{1}{2}, \frac{1}{2}\right]$ | [1,2,3,4,13,14,21,22,25,26,27,28,37,38,45,46] |
| 2 | $\left[\frac{1}{2}, 0, \frac{1}{2}\right]$ | [5,8,10,12,17,18,19,20,29,32,34,36,41,42,43,44] |
| 3 | $\left[\frac{1}{2}, \frac{1}{2}, 0\right]$ | [6,7,9,11,15,16,23,24,30,31,33,35,39,40,47,48] |

Table 4: Wyckoff site: `3d`, site symmetry: `-42.m1'`

| No. | position | mapping |
|---|---|---|
| 1 | $\left[\frac{1}{2}, 0, 0\right]$ | [1,2,3,4,13,14,21,22,25,26,27,28,37,38,45,46] |
| 2 | $\left[0, \frac{1}{2}, 0\right]$ | [5,8,10,12,17,18,19,20,29,32,34,36,41,42,43,44] |
| 3 | $\left[0, 0, \frac{1}{2}\right]$ | [6,7,9,11,15,16,23,24,30,31,33,35,39,40,47,48] |

Table 5: Wyckoff site: `4e`, site symmetry: `.3m1'`

| No. | position | mapping |
|---|---|---|
| 1 | $[x, x, x]$ | [1,5,6,20,22,24,25,29,30,44,46,48] |
| 2 | $[x, -x, -x]$ | [2,10,11,16,17,21,26,34,35,40,41,45] |
| 3 | $[-x, x, -x]$ | [3,7,12,13,18,23,27,31,36,37,42,47] |
| 4 | $[-x, -x, x]$ | [4,8,9,14,15,19,28,32,33,38,39,43] |

Table 6: Wyckoff site: `6f`, site symmetry: `2.mm1'`

| No. | position | mapping |
|---|---|---|
| 1 | $[x,\ 0,\ 0]$ | `[1,2,21,22,25,26,45,46]` |
| 2 | $[-x,\ 0,\ 0]$ | `[3,4,13,14,27,28,37,38]` |
| 3 | $[0,\ x,\ 0]$ | `[5,12,18,20,29,36,42,44]` |
| 4 | $[0,\ 0,\ x]$ | `[6,9,15,24,30,33,39,48]` |
| 5 | $[0,\ 0,\ -x]$ | `[7,11,16,23,31,35,40,47]` |
| 6 | $[0,\ -x,\ 0]$ | `[8,10,17,19,32,34,41,43]` |

Table 7: Wyckoff site: `6g`, site symmetry: `2.mm1'`

| No. | position | mapping |
|---|---|---|
| 1 | $\left[x,\ \frac{1}{2},\ \frac{1}{2}\right]$ | `[1,2,21,22,25,26,45,46]` |
| 2 | $\left[-x,\ \frac{1}{2},\ \frac{1}{2}\right]$ | `[3,4,13,14,27,28,37,38]` |
| 3 | $\left[\frac{1}{2},\ x,\ \frac{1}{2}\right]$ | `[5,12,18,20,29,36,42,44]` |
| 4 | $\left[\frac{1}{2},\ \frac{1}{2},\ x\right]$ | `[6,9,15,24,30,33,39,48]` |
| 5 | $\left[\frac{1}{2},\ \frac{1}{2},\ -x\right]$ | `[7,11,16,23,31,35,40,47]` |
| 6 | $\left[\frac{1}{2},\ -x,\ \frac{1}{2}\right]$ | `[8,10,17,19,32,34,41,43]` |

Table 8: Wyckoff site: `12h`, site symmetry: `2..1'`

| No. | position | mapping |
|---|---|---|
| 1 | $\left[x,\ \frac{1}{2},\ 0\right]$ | `[1,2,25,26]` |
| 2 | $\left[-x,\ \frac{1}{2},\ 0\right]$ | `[3,4,27,28]` |
| 3 | $\left[0,\ x,\ \frac{1}{2}\right]$ | `[5,12,29,36]` |
| 4 | $\left[\frac{1}{2},\ 0,\ x\right]$ | `[6,9,30,33]` |
| 5 | $\left[\frac{1}{2},\ 0,\ -x\right]$ | `[7,11,31,35]` |
| 6 | $\left[0,\ -x,\ \frac{1}{2}\right]$ | `[8,10,32,34]` |
| 7 | $\left[-x,\ 0,\ \frac{1}{2}\right]$ | `[13,14,37,38]` |
| 8 | $\left[0,\ \frac{1}{2},\ x\right]$ | `[15,24,39,48]` |
| 9 | $\left[0,\ \frac{1}{2},\ -x\right]$ | `[16,23,40,47]` |
| 10 | $\left[\frac{1}{2},\ -x,\ 0\right]$ | `[17,19,41,43]` |
| 11 | $\left[\frac{1}{2},\ x,\ 0\right]$ | `[18,20,42,44]` |
| 12 | $\left[x,\ 0,\ \frac{1}{2}\right]$ | `[21,22,45,46]` |

Table 9: Wyckoff site: `12i`, site symmetry: `..m1'`

| No. | position | mapping |
|---|---|---|
| 1 | $[x,\ x,\ z]$ | `[1,20,25,44]` |
| 2 | $[x,\ -x,\ -z]$ | `[2,17,26,41]` |
| 3 | $[-x,\ x,\ -z]$ | `[3,18,27,42]` |

*continued ...*

Table 9

| No. | position | mapping |
|---|---|---|
| 4 | $[-x, -x, z]$ | [4,19,28,43] |
| 5 | $[z, x, x]$ | [5,24,29,48] |
| 6 | $[x, z, x]$ | [6,22,30,46] |
| 7 | $[-x, z, -x]$ | [7,13,31,37] |
| 8 | $[-z, -x, x]$ | [8,15,32,39] |
| 9 | $[-x, -z, x]$ | [9,14,33,38] |
| 10 | $[z, -x, -x]$ | [10,16,34,40] |
| 11 | $[x, -z, -x]$ | [11,21,35,45] |
| 12 | $[-z, x, -x]$ | [12,23,36,47] |

Table 10: Wyckoff site: 24j, site symmetry: 11'

| No. | position | mapping |
|---|---|---|
| 1 | $[x, y, z]$ | [1,25] |
| 2 | $[x, -y, -z]$ | [2,26] |
| 3 | $[-x, y, -z]$ | [3,27] |
| 4 | $[-x, -y, z]$ | [4,28] |
| 5 | $[z, x, y]$ | [5,29] |
| 6 | $[y, z, x]$ | [6,30] |
| 7 | $[-y, z, -x]$ | [7,31] |
| 8 | $[-z, -x, y]$ | [8,32] |
| 9 | $[-y, -z, x]$ | [9,33] |
| 10 | $[z, -x, -y]$ | [10,34] |
| 11 | $[y, -z, -x]$ | [11,35] |
| 12 | $[-z, x, -y]$ | [12,36] |
| 13 | $[-x, z, -y]$ | [13,37] |
| 14 | $[-x, -z, y]$ | [14,38] |
| 15 | $[-z, -y, x]$ | [15,39] |
| 16 | $[z, -y, -x]$ | [16,40] |
| 17 | $[y, -x, -z]$ | [17,41] |
| 18 | $[-y, x, -z]$ | [18,42] |
| 19 | $[-y, -x, z]$ | [19,43] |
| 20 | $[y, x, z]$ | [20,44] |
| 21 | $[x, -z, -y]$ | [21,45] |
| 22 | $[x, z, y]$ | [22,46] |
| 23 | $[-z, y, -x]$ | [23,47] |
| 24 | $[z, y, x]$ | [24,48] |