# MSG No. 134.472 $P4_2/nnm1'$ [ Type II, tetragonal ]

Table 1: Wyckoff site: `2a`, site symmetry: `-42m1'`

| No. | position | mapping |
|---|---|---|
| 1 | $\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}\right]$ | `[1,4,5,6,10,11,15,16,17,20,21,22,26,27,31,32]` |
| 2 | $\left[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}\right]$ | `[2,3,7,8,9,12,13,14,18,19,23,24,25,28,29,30]` |

Table 2: Wyckoff site: `2b`, site symmetry: `-42m1'`

| No. | position | mapping |
|---|---|---|
| 1 | $\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right]$ | `[1,4,5,6,10,11,15,16,17,20,21,22,26,27,31,32]` |
| 2 | $\left[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}\right]$ | `[2,3,7,8,9,12,13,14,18,19,23,24,25,28,29,30]` |

Table 3: Wyckoff site: `4c`, site symmetry: `222.1'`

| No. | position | mapping |
|---|---|---|
| 1 | $\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$ | `[1,4,5,6,17,20,21,22]` |
| 2 | $\left[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}\right]$ | `[2,3,7,8,18,19,23,24]` |
| 3 | $\left[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right]$ | `[9,12,13,14,25,28,29,30]` |
| 4 | $\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}\right]$ | `[10,11,15,16,26,27,31,32]` |

Table 4: Wyckoff site: `4d`, site symmetry: `2.221'`

| No. | position | mapping |
|---|---|---|
| 1 | $\left[\frac{1}{4}, \frac{1}{4}, 0\right]$ | `[1,6,7,8,17,22,23,24]` |
| 2 | $\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}\right]$ | `[2,3,4,5,18,19,20,21]` |
| 3 | $\left[\frac{3}{4}, \frac{3}{4}, 0\right]$ | `[9,14,15,16,25,30,31,32]` |
| 4 | $\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}\right]$ | `[10,11,12,13,26,27,28,29]` |

Table 5: Wyckoff site: `4e`, site symmetry: `..2/m1'`

| No. | position | mapping |
|---|---|---|
| 1 | $\left[0, 0, \frac{1}{2}\right]$ | `[1,7,9,15,17,23,25,31]` |
| 2 | $\left[\frac{1}{2}, 0, 0\right]$ | `[2,5,10,13,18,21,26,29]` |
| 3 | $\left[0, \frac{1}{2}, 0\right]$ | `[3,4,11,12,19,20,27,28]` |
| 4 | $\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$ | `[6,8,14,16,22,24,30,32]` |

Table 6: Wyckoff site: `4f`, site symmetry: `..2/m1'`

| No. | position | mapping |
|---|---|---|
| 1 | $[0,\ 0,\ 0]$ | `[1,7,9,15,17,23,25,31]` |
| 2 | $\left[\frac{1}{2},\ 0,\ \frac{1}{2}\right]$ | `[2,5,10,13,18,21,26,29]` |
| 3 | $\left[0,\ \frac{1}{2},\ \frac{1}{2}\right]$ | `[3,4,11,12,19,20,27,28]` |
| 4 | $\left[\frac{1}{2},\ \frac{1}{2},\ 0\right]$ | `[6,8,14,16,22,24,30,32]` |

Table 7: Wyckoff site: `4g`, site symmetry: `2.mm1'`

| No. | position | mapping |
|---|---|---|
| 1 | $\left[\frac{3}{4},\ \frac{1}{4},\ z\right]$ | `[1,6,15,16,17,22,31,32]` |
| 2 | $\left[\frac{1}{4},\ \frac{3}{4},\ z+\frac{1}{2}\right]$ | `[2,3,12,13,18,19,28,29]` |
| 3 | $\left[\frac{3}{4},\ \frac{1}{4},\ \frac{1}{2}-z\right]$ | `[4,5,10,11,20,21,26,27]` |
| 4 | $\left[\frac{1}{4},\ \frac{3}{4},\ -z\right]$ | `[7,8,9,14,23,24,25,30]` |

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

| No. | position | mapping |
|---|---|---|
| 1 | $\left[\frac{1}{4},\ \frac{1}{4},\ z\right]$ | `[1,6,17,22]` |
| 2 | $\left[\frac{1}{4},\ \frac{1}{4},\ z+\frac{1}{2}\right]$ | `[2,3,18,19]` |
| 3 | $\left[\frac{1}{4},\ \frac{1}{4},\ \frac{1}{2}-z\right]$ | `[4,5,20,21]` |
| 4 | $\left[\frac{1}{4},\ \frac{1}{4},\ -z\right]$ | `[7,8,23,24]` |
| 5 | $\left[\frac{3}{4},\ \frac{3}{4},\ -z\right]$ | `[9,14,25,30]` |
| 6 | $\left[\frac{3}{4},\ \frac{3}{4},\ \frac{1}{2}-z\right]$ | `[10,11,26,27]` |
| 7 | $\left[\frac{3}{4},\ \frac{3}{4},\ z+\frac{1}{2}\right]$ | `[12,13,28,29]` |
| 8 | $\left[\frac{3}{4},\ \frac{3}{4},\ z\right]$ | `[15,16,31,32]` |

Table 9: Wyckoff site: `8i`, site symmetry: `.2.1'`

| No. | position | mapping |
|---|---|---|
| 1 | $\left[x,\ \frac{1}{4},\ \frac{3}{4}\right]$ | `[1,4,17,20]` |
| 2 | $\left[\frac{1}{4},\ x,\ \frac{1}{4}\right]$ | `[2,7,18,23]` |
| 3 | $\left[\frac{1}{4},\ \frac{1}{2}-x,\ \frac{1}{4}\right]$ | `[3,8,19,24]` |
| 4 | $\left[\frac{1}{2}-x,\ \frac{1}{4},\ \frac{3}{4}\right]$ | `[5,6,21,22]` |
| 5 | $\left[-x,\ \frac{3}{4},\ \frac{1}{4}\right]$ | `[9,12,25,28]` |
| 6 | $\left[\frac{3}{4},\ -x,\ \frac{3}{4}\right]$ | `[10,15,26,31]` |
| 7 | $\left[\frac{3}{4},\ x+\frac{1}{2},\ \frac{3}{4}\right]$ | `[11,16,27,32]` |
| 8 | $\left[x+\frac{1}{2},\ \frac{3}{4},\ \frac{1}{4}\right]$ | `[13,14,29,30]` |

Table 10: Wyckoff site: 8j, site symmetry: .2.1'

| No. | position | mapping |
|---|---|---|
| 1 | $\left[x,\ \frac{1}{4},\ \frac{1}{4}\right]$ | [1,4,17,20] |
| 2 | $\left[\frac{1}{4},\ x,\ \frac{3}{4}\right]$ | [2,7,18,23] |
| 3 | $\left[\frac{1}{4},\ \frac{1}{2}-x,\ \frac{3}{4}\right]$ | [3,8,19,24] |
| 4 | $\left[\frac{1}{2}-x,\ \frac{1}{4},\ \frac{1}{4}\right]$ | [5,6,21,22] |
| 5 | $\left[-x,\ \frac{3}{4},\ \frac{3}{4}\right]$ | [9,12,25,28] |
| 6 | $\left[\frac{3}{4},\ -x,\ \frac{1}{4}\right]$ | [10,15,26,31] |
| 7 | $\left[\frac{3}{4},\ x+\frac{1}{2},\ \frac{1}{4}\right]$ | [11,16,27,32] |
| 8 | $\left[x+\frac{1}{2},\ \frac{3}{4},\ \frac{3}{4}\right]$ | [13,14,29,30] |

Table 11: Wyckoff site: 8k, site symmetry: ..21'

| No. | position | mapping |
|---|---|---|
| 1 | $[x,\ x,\ 0]$ | [1,7,17,23] |
| 2 | $\left[\frac{1}{2}-x,\ x,\ \frac{1}{2}\right]$ | [2,5,18,21] |
| 3 | $\left[x,\ \frac{1}{2}-x,\ \frac{1}{2}\right]$ | [3,4,19,20] |
| 4 | $\left[\frac{1}{2}-x,\ \frac{1}{2}-x,\ 0\right]$ | [6,8,22,24] |
| 5 | $[-x,\ -x,\ 0]$ | [9,15,25,31] |
| 6 | $\left[x+\frac{1}{2},\ -x,\ \frac{1}{2}\right]$ | [10,13,26,29] |
| 7 | $\left[-x,\ x+\frac{1}{2},\ \frac{1}{2}\right]$ | [11,12,27,28] |
| 8 | $\left[x+\frac{1}{2},\ x+\frac{1}{2},\ 0\right]$ | [14,16,30,32] |

Table 12: Wyckoff site: 8l, site symmetry: ..21'

| No. | position | mapping |
|---|---|---|
| 1 | $\left[x,\ x,\ \frac{1}{2}\right]$ | [1,7,17,23] |
| 2 | $\left[\frac{1}{2}-x,\ x,\ 0\right]$ | [2,5,18,21] |
| 3 | $\left[x,\ \frac{1}{2}-x,\ 0\right]$ | [3,4,19,20] |
| 4 | $\left[\frac{1}{2}-x,\ \frac{1}{2}-x,\ \frac{1}{2}\right]$ | [6,8,22,24] |
| 5 | $\left[-x,\ -x,\ \frac{1}{2}\right]$ | [9,15,25,31] |
| 6 | $\left[x+\frac{1}{2},\ -x,\ 0\right]$ | [10,13,26,29] |
| 7 | $\left[-x,\ x+\frac{1}{2},\ 0\right]$ | [11,12,27,28] |
| 8 | $\left[x+\frac{1}{2},\ x+\frac{1}{2},\ \frac{1}{2}\right]$ | [14,16,30,32] |

Table 13: Wyckoff site: 8m, site symmetry: ..m1'

| No. | position | mapping |
|---|---|---|
| 1 | $[x,\ -x,\ z]$ | [1,15,17,31] |
| 2 | $\left[x+\frac{1}{2},\ x,\ z+\frac{1}{2}\right]$ | [2,13,18,29] |
| 3 | $\left[-x,\ \frac{1}{2}-x,\ z+\frac{1}{2}\right]$ | [3,12,19,28] |

*continued ...*

Table 13

| No. | position | mapping |
|---|---|---|
| 4 | $\left[x,\, x+\frac{1}{2},\, \frac{1}{2}-z\right]$ | `[4,11,20,27]` |
| 5 | $\left[\frac{1}{2}-x,\, -x,\, \frac{1}{2}-z\right]$ | `[5,10,21,26]` |
| 6 | $\left[\frac{1}{2}-x,\, x+\frac{1}{2},\, z\right]$ | `[6,16,22,32]` |
| 7 | $[-x,\, x,\, -z]$ | `[7,9,23,25]` |
| 8 | $\left[x+\frac{1}{2},\, \frac{1}{2}-x,\, -z\right]$ | `[8,14,24,30]` |

Table 14: Wyckoff site: `16n`, site symmetry: `11'`

| No. | position | mapping |
|---|---|---|
| 1 | $[x,\, y,\, z]$ | `[1,17]` |
| 2 | $\left[\frac{1}{2}-y,\, x,\, z+\frac{1}{2}\right]$ | `[2,18]` |
| 3 | $\left[y,\, \frac{1}{2}-x,\, z+\frac{1}{2}\right]$ | `[3,19]` |
| 4 | $\left[x,\, \frac{1}{2}-y,\, \frac{1}{2}-z\right]$ | `[4,20]` |
| 5 | $\left[\frac{1}{2}-x,\, y,\, \frac{1}{2}-z\right]$ | `[5,21]` |
| 6 | $\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, z\right]$ | `[6,22]` |
| 7 | $[y,\, x,\, -z]$ | `[7,23]` |
| 8 | $\left[\frac{1}{2}-y,\, \frac{1}{2}-x,\, -z\right]$ | `[8,24]` |
| 9 | $[-x,\, -y,\, -z]$ | `[9,25]` |
| 10 | $\left[y+\frac{1}{2},\, -x,\, \frac{1}{2}-z\right]$ | `[10,26]` |
| 11 | $\left[-y,\, x+\frac{1}{2},\, \frac{1}{2}-z\right]$ | `[11,27]` |
| 12 | $\left[-x,\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$ | `[12,28]` |
| 13 | $\left[x+\frac{1}{2},\, -y,\, z+\frac{1}{2}\right]$ | `[13,29]` |
| 14 | $\left[x+\frac{1}{2},\, y+\frac{1}{2},\, -z\right]$ | `[14,30]` |
| 15 | $[-y,\, -x,\, z]$ | `[15,31]` |
| 16 | $\left[y+\frac{1}{2},\, x+\frac{1}{2},\, z\right]$ | `[16,32]` |