# MSG No. 124.361 $P_C4/mcc$ [ Type IV, tetragonal ]

Table 1: Wyckoff site: `4a`, site symmetry: `422`

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

Table 2: Wyckoff site: `4b`, site symmetry: `4/m..`

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

Table 3: Wyckoff site: `4c`, site symmetry: `4'22'`

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

Table 4: Wyckoff site: `4d`, site symmetry: `4'/m..`

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

Table 5: Wyckoff site: `8e`, site symmetry: `2'/m..`

| No. | position | mapping |
|---|---|---|
| 1 | $\left[\frac{3}{4},\ \frac{1}{4},\ 0\right]$ | `[1,14,22,25]` |
| 2 | $\left[\frac{3}{4},\ \frac{3}{4},\ 0\right]$ | `[2,11,19,26]` |

*continued ...*

Table 5

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

Table 6: Wyckoff site: 8f, site symmetry: 2.22

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

Table 7: Wyckoff site: 8g, site symmetry: 4..

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

Table 8: Wyckoff site: 8h, site symmetry: 4'..

| No. | position | mapping |
|---|---|---|
| 1 | $\left[0, \frac{1}{2}, z\right]$ | [1,6,18,19] |
| 2 | $\left[\frac{1}{2}, 0, z\right]$ | [2,3,17,22] |
| 3 | $\left[0, \frac{1}{2}, \frac{1}{2} - z\right]$ | [4,5,23,24] |
| 4 | $\left[\frac{1}{2}, 0, \frac{1}{2} - z\right]$ | [7,8,20,21] |
| 5 | $\left[0, \frac{1}{2}, -z\right]$ | [9,14,26,27] |

*continued ...*

Table 8

| No. | position | mapping |
|---|---|---|
| 6 | $\left[\frac{1}{2}, 0, -z\right]$ | [10,11,25,30] |
| 7 | $\left[0, \frac{1}{2}, z+\frac{1}{2}\right]$ | [12,13,31,32] |
| 8 | $\left[\frac{1}{2}, 0, z+\frac{1}{2}\right]$ | [15,16,28,29] |

Table 9: Wyckoff site: 16i, site symmetry: 2'..

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

Table 10: Wyckoff site: 16j, site symmetry: .2.

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

*continued ...*

Table 10

| No. | position | mapping |
|---|---|---|
| 16 | $\left[\frac{1}{2}, y+\frac{1}{2}, \frac{3}{4}\right]$ | [28,30] |

Table 11: Wyckoff site: 16k, site symmetry: ..2

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

Table 12: Wyckoff site: 16l, site symmetry: ..2'

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

Table 13: Wyckoff site: `16m`, site symmetry: `m..`

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

Table 14: Wyckoff site: `32n`, site symmetry: `1`

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

*continued ...*

Table 14

| No. | position | mapping |
|---|---|---|
| 24 | $\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ \frac{1}{2}-z\right]$ | [24] |
| 25 | $\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ -z\right]$ | [25] |
| 26 | $\left[y+\frac{1}{2},\ \frac{1}{2}-x,\ -z\right]$ | [26] |
| 27 | $\left[\frac{1}{2}-y,\ x+\frac{1}{2},\ -z\right]$ | [27] |
| 28 | $\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$ | [28] |
| 29 | $\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$ | [29] |
| 30 | $\left[x+\frac{1}{2},\ y+\frac{1}{2},\ -z\right]$ | [30] |
| 31 | $\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ z+\frac{1}{2}\right]$ | [31] |
| 32 | $\left[y+\frac{1}{2},\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$ | [32] |