# MSG No. 130.433 $P_C4/ncc$ [ Type IV, tetragonal ]

Table 1: Wyckoff site: `4a`, site symmetry: `42'2'`

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

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

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

Table 3: Wyckoff site: `4c`, site symmetry: `4'2'2`

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

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

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

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

| No. | position | mapping |
|---|---|---|
| 1 | $\left[\frac{1}{2}, 0, 0\right]$ | `[1,9,22,30]` |
| 2 | $\left[\frac{1}{2}, \frac{1}{2}, 0\right]$ | `[2,10,19,27]` |

*continued ...*

Table 5

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

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

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

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

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

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

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

*continued ...*

Table 8

| No. | position | mapping |
|---|---|---|
| 6 | $\left[\frac{3}{4}, \frac{1}{4}, -z\right]$ | [10,11,25,30] |
| 7 | $\left[\frac{3}{4}, \frac{1}{4}, z+\frac{1}{2}\right]$ | [12,13,31,32] |
| 8 | $\left[\frac{1}{4}, \frac{3}{4}, z+\frac{1}{2}\right]$ | [15,16,28,29] |

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

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

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

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

*continued ...*

Table 10

| No. | position | mapping |
|---|---|---|
| 16 | $\left[y,\ \frac{3}{4},\ \frac{3}{4}\right]$ | [16,26] |

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

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

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

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

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

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

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

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