# MSG No. 142.561 $I4_1/acd$ [ Type I, tetragonal ]

Table 1: Wyckoff site: `8a`, site symmetry: `-4..`

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

Table 2: Wyckoff site: `8b`, site symmetry: `2.22`

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

Table 3: Wyckoff site: `16c`, site symmetry: `-1`

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

*continued ...*

Table 3

| No. | position | mapping |
|---|---|---|
| 16 | $\left[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right]$ | [24,32] |

Table 4: Wyckoff site: 16d, site symmetry: 2..

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

Table 5: Wyckoff site: 16e, site symmetry: .2.

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

Table 6: Wyckoff site: 16f, site symmetry: ..2

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

Table 7: Wyckoff site: 32g, site symmetry: 1

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

*continued ...*

Table 7

| No. | position | mapping |
|-----|----------|---------|
| 24 | $\left[\frac{3}{4} - y,\ \frac{3}{4} - x,\ \frac{3}{4} - z\right]$ | [24] |
| 25 | $\left[\frac{1}{2} - x,\ \frac{1}{2} - y,\ \frac{1}{2} - z\right]$ | [25] |
| 26 | $\left[y + \frac{1}{4},\ \frac{3}{4} - x,\ \frac{1}{4} - z\right]$ | [26] |
| 27 | $\left[\frac{3}{4} - y,\ x + \frac{3}{4},\ \frac{1}{4} - z\right]$ | [27] |
| 28 | $\left[\frac{1}{2} - x,\ y + \frac{1}{2},\ z\right]$ | [28] |
| 29 | $\left[x + \frac{1}{2},\ -y,\ z\right]$ | [29] |
| 30 | $\left[x + \frac{1}{2},\ y,\ \frac{1}{2} - z\right]$ | [30] |
| 31 | $\left[\frac{1}{4} - y,\ \frac{3}{4} - x,\ z + \frac{3}{4}\right]$ | [31] |
| 32 | $\left[y + \frac{3}{4},\ x + \frac{3}{4},\ z + \frac{3}{4}\right]$ | [32] |