# MSG No. 221.92 $Pm\bar{3}m$ [ Type I, cubic ]

Table 1: Wyckoff site: 1a, site symmetry: m-3m

| 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: m-3m

| 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: 4/mm.m

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

Table 4: Wyckoff site: 3d, site symmetry: 4/mm.m

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

Table 5: Wyckoff site: 6e, site symmetry: 4m.m

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

Table 6: Wyckoff site: `6f`, site symmetry: `4m.m`

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

Table 7: Wyckoff site: `8g`, site symmetry: `.3m`

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

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

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

Table 9: Wyckoff site: `12i`, site symmetry: `m.2m`

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

Table 10: Wyckoff site: `12j`, site symmetry: `m.2m`

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

Table 11: Wyckoff site: `24k`, site symmetry: `m..`

| No. | position | mapping |
|---|---|---|
| 1 | $[0,\ y,\ z]$ | `[1,32]` |
| 2 | $[0,\ -z,\ y]$ | `[2,27]` |
| 3 | $[0,\ z,\ -y]$ | `[3,26]` |
| 4 | $[z,\ y,\ 0]$ | `[4,40]` |
| 5 | $[-z,\ y,\ 0]$ | `[5,39]` |
| 6 | $[-y,\ 0,\ z]$ | `[6,35]` |
| 7 | $[y,\ 0,\ z]$ | `[7,36]` |
| 8 | $[0,\ -y,\ -z]$ | `[8,25]` |
| 9 | $[0,\ y,\ -z]$ | `[9,34]` |

*continued ...*

Table 11

| No. | position | mapping |
|---|---|---|
| 10 | $[0, -y, z]$ | [10,33] |
| 11 | $[y, 0, -z]$ | [11,30] |
| 12 | $[-y, 0, -z]$ | [12,31] |
| 13 | $[0, z, y]$ | [13,38] |
| 14 | $[0, -z, -y]$ | [14,37] |
| 15 | $[z, -y, 0]$ | [15,29] |
| 16 | $[-z, -y, 0]$ | [16,28] |
| 17 | $[z, 0, y]$ | [17,48] |
| 18 | $[y, z, 0]$ | [18,45] |
| 19 | $[-y, z, 0]$ | [19,47] |
| 20 | $[-z, 0, y]$ | [20,46] |
| 21 | $[-y, -z, 0]$ | [21,42] |
| 22 | $[z, 0, -y]$ | [22,44] |
| 23 | $[y, -z, 0]$ | [23,43] |
| 24 | $[-z, 0, -y]$ | [24,41] |

Table 12: Wyckoff site: 24l, site symmetry: m..

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

Table 13: Wyckoff site: `24m`, site symmetry: `..m`

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

Table 14: Wyckoff site: `48n`, site symmetry: `1`

| No. | position | mapping |
|---|---|---|
| 1 | $[x, y, z]$ | `[1]` |
| 2 | $[x, -z, y]$ | `[2]` |
| 3 | $[x, z, -y]$ | `[3]` |
| 4 | $[z, y, -x]$ | `[4]` |
| 5 | $[-z, y, x]$ | `[5]` |
| 6 | $[-y, x, z]$ | `[6]` |
| 7 | $[y, -x, z]$ | `[7]` |
| 8 | $[x, -y, -z]$ | `[8]` |
| 9 | $[-x, y, -z]$ | `[9]` |
| 10 | $[-x, -y, z]$ | `[10]` |
| 11 | $[y, x, -z]$ | `[11]` |
| 12 | $[-y, -x, -z]$ | `[12]` |
| 13 | $[-x, z, y]$ | `[13]` |
| 14 | $[-x, -z, -y]$ | `[14]` |
| 15 | $[z, -y, x]$ | `[15]` |

*continued ...*

Table 14

| No. | position | mapping |
|---|---|---|
| 16 | $[-z, -y, -x]$ | [16] |
| 17 | $[z, x, y]$ | [17] |
| 18 | $[y, z, x]$ | [18] |
| 19 | $[-y, z, -x]$ | [19] |
| 20 | $[-z, -x, y]$ | [20] |
| 21 | $[-y, -z, x]$ | [21] |
| 22 | $[z, -x, -y]$ | [22] |
| 23 | $[y, -z, -x]$ | [23] |
| 24 | $[-z, x, -y]$ | [24] |
| 25 | $[-x, -y, -z]$ | [25] |
| 26 | $[-x, z, -y]$ | [26] |
| 27 | $[-x, -z, y]$ | [27] |
| 28 | $[-z, -y, x]$ | [28] |
| 29 | $[z, -y, -x]$ | [29] |
| 30 | $[y, -x, -z]$ | [30] |
| 31 | $[-y, x, -z]$ | [31] |
| 32 | $[-x, y, z]$ | [32] |
| 33 | $[x, -y, z]$ | [33] |
| 34 | $[x, y, -z]$ | [34] |
| 35 | $[-y, -x, z]$ | [35] |
| 36 | $[y, x, z]$ | [36] |
| 37 | $[x, -z, -y]$ | [37] |
| 38 | $[x, z, y]$ | [38] |
| 39 | $[-z, y, -x]$ | [39] |
| 40 | $[z, y, x]$ | [40] |
| 41 | $[-z, -x, -y]$ | [41] |
| 42 | $[-y, -z, -x]$ | [42] |
| 43 | $[y, -z, x]$ | [43] |
| 44 | $[z, x, -y]$ | [44] |
| 45 | $[y, z, -x]$ | [45] |
| 46 | $[-z, x, y]$ | [46] |
| 47 | $[-y, z, x]$ | [47] |
| 48 | $[z, -x, y]$ | [48] |