# MSG No. 196.4 $F23$ [ Type I, cubic ]

Table 1: Wyckoff site: `4a`, site symmetry: `23.`

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

Table 2: Wyckoff site: `4b`, site symmetry: `23.`

| 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]` |
| 2 | $\left[\frac{1}{2}, 0, 0\right]$ | `[13,14,15,16,17,18,19,20,21,22,23,24]` |
| 3 | $\left[0, \frac{1}{2}, 0\right]$ | `[25,26,27,28,29,30,31,32,33,34,35,36]` |
| 4 | $\left[0, 0, \frac{1}{2}\right]$ | `[37,38,39,40,41,42,43,44,45,46,47,48]` |

Table 3: Wyckoff site: `4c`, site symmetry: `23.`

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

Table 4: Wyckoff site: `4d`, site symmetry: `23.`

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

Table 5: Wyckoff site: `16e`, site symmetry: `.3.`

| No. | position | mapping |
|---|---|---|
| 1 | $[x, x, x]$ | `[1,5,6]` |
| 2 | $[x, -x, -x]$ | `[2,10,11]` |

*continued ...*

Table 5

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

Table 6: Wyckoff site: `24f`, site symmetry: `2..`

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

Table 7: Wyckoff site: 24g, site symmetry: 2..

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

Table 8: Wyckoff site: 48h, site symmetry: 1

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

*continued ...*

Table 8

| No. | position | mapping |
|---|---|---|
| 16 | $\left[-x,\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$ | [16] |
| 17 | $\left[z,\ x+\frac{1}{2},\ y+\frac{1}{2}\right]$ | [17] |
| 18 | $\left[y,\ z+\frac{1}{2},\ x+\frac{1}{2}\right]$ | [18] |
| 19 | $\left[-y,\ z+\frac{1}{2},\ \frac{1}{2}-x\right]$ | [19] |
| 20 | $\left[-z,\ \frac{1}{2}-x,\ y+\frac{1}{2}\right]$ | [20] |
| 21 | $\left[-y,\ \frac{1}{2}-z,\ x+\frac{1}{2}\right]$ | [21] |
| 22 | $\left[z,\ \frac{1}{2}-x,\ \frac{1}{2}-y\right]$ | [22] |
| 23 | $\left[y,\ \frac{1}{2}-z,\ \frac{1}{2}-x\right]$ | [23] |
| 24 | $\left[-z,\ x+\frac{1}{2},\ \frac{1}{2}-y\right]$ | [24] |
| 25 | $\left[x+\frac{1}{2},\ y,\ z+\frac{1}{2}\right]$ | [25] |
| 26 | $\left[x+\frac{1}{2},\ -y,\ \frac{1}{2}-z\right]$ | [26] |
| 27 | $\left[\frac{1}{2}-x,\ y,\ \frac{1}{2}-z\right]$ | [27] |
| 28 | $\left[\frac{1}{2}-x,\ -y,\ z+\frac{1}{2}\right]$ | [28] |
| 29 | $\left[z+\frac{1}{2},\ x,\ y+\frac{1}{2}\right]$ | [29] |
| 30 | $\left[y+\frac{1}{2},\ z,\ x+\frac{1}{2}\right]$ | [30] |
| 31 | $\left[\frac{1}{2}-y,\ z,\ \frac{1}{2}-x\right]$ | [31] |
| 32 | $\left[\frac{1}{2}-z,\ -x,\ y+\frac{1}{2}\right]$ | [32] |
| 33 | $\left[\frac{1}{2}-y,\ -z,\ x+\frac{1}{2}\right]$ | [33] |
| 34 | $\left[z+\frac{1}{2},\ -x,\ \frac{1}{2}-y\right]$ | [34] |
| 35 | $\left[y+\frac{1}{2},\ -z,\ \frac{1}{2}-x\right]$ | [35] |
| 36 | $\left[\frac{1}{2}-z,\ x,\ \frac{1}{2}-y\right]$ | [36] |
| 37 | $\left[x+\frac{1}{2},\ y+\frac{1}{2},\ z\right]$ | [37] |
| 38 | $\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ -z\right]$ | [38] |
| 39 | $\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ -z\right]$ | [39] |
| 40 | $\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ z\right]$ | [40] |
| 41 | $\left[z+\frac{1}{2},\ x+\frac{1}{2},\ y\right]$ | [41] |
| 42 | $\left[y+\frac{1}{2},\ z+\frac{1}{2},\ x\right]$ | [42] |
| 43 | $\left[\frac{1}{2}-y,\ z+\frac{1}{2},\ -x\right]$ | [43] |
| 44 | $\left[\frac{1}{2}-z,\ \frac{1}{2}-x,\ y\right]$ | [44] |
| 45 | $\left[\frac{1}{2}-y,\ \frac{1}{2}-z,\ x\right]$ | [45] |
| 46 | $\left[z+\frac{1}{2},\ \frac{1}{2}-x,\ -y\right]$ | [46] |
| 47 | $\left[y+\frac{1}{2},\ \frac{1}{2}-z,\ -x\right]$ | [47] |
| 48 | $\left[\frac{1}{2}-z,\ x+\frac{1}{2},\ -y\right]$ | [48] |