# MSG No. 196.5 $F231'$ [ Type II, cubic ]

Table 1: Wyckoff site: 4a, site symmetry: 23.1'

| No. | position | mapping |
|---|---|---|
| 1 | $[0,\ 0,\ 0]$ | [1,2,3,4,5,6,7,8,9,10,11,12,49,50,51,52,53,54,55,56,57,58,59,60] |
| 2 | $\left[0,\ \frac{1}{2},\ \frac{1}{2}\right]$ | [13,14,15,16,17,18,19,20,21,22,23,24,61,62,63,64,65,66,67,68,69,70,71,72] |
| 3 | $\left[\frac{1}{2},\ 0,\ \frac{1}{2}\right]$ | [25,26,27,28,29,30,31,32,33,34,35,36,73,74,75,76,77,78,79,80,81,82,83,84] |
| 4 | $\left[\frac{1}{2},\ \frac{1}{2},\ 0\right]$ | [37,38,39,40,41,42,43,44,45,46,47,48,85,86,87,88,89,90,91,92,93,94,95,96] |

Table 2: Wyckoff site: 4b, site symmetry: 23.1'

| No. | position | mapping |
|---|---|---|
| 1 | $\left[\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}\right]$ | [1,2,3,4,5,6,7,8,9,10,11,12,49,50,51,52,53,54,55,56,57,58,59,60] |
| 2 | $\left[\frac{1}{2},\ 0,\ 0\right]$ | [13,14,15,16,17,18,19,20,21,22,23,24,61,62,63,64,65,66,67,68,69,70,71,72] |
| 3 | $\left[0,\ \frac{1}{2},\ 0\right]$ | [25,26,27,28,29,30,31,32,33,34,35,36,73,74,75,76,77,78,79,80,81,82,83,84] |
| 4 | $\left[0,\ 0,\ \frac{1}{2}\right]$ | [37,38,39,40,41,42,43,44,45,46,47,48,85,86,87,88,89,90,91,92,93,94,95,96] |

Table 3: Wyckoff site: 4c, site symmetry: 23.1'

| No. | position | mapping |
|---|---|---|
| 1 | $\left[\frac{1}{4},\ \frac{1}{4},\ \frac{1}{4}\right]$ | [1,5,6,14,22,23,27,31,36,40,44,45,49,53,54,62,70,71,75,79,84,88,92,93] |
| 2 | $\left[\frac{1}{4},\ \frac{3}{4},\ \frac{3}{4}\right]$ | [2,10,11,13,17,18,28,32,33,39,43,48,50,58,59,61,65,66,76,80,81,87,91,96] |
| 3 | $\left[\frac{3}{4},\ \frac{1}{4},\ \frac{3}{4}\right]$ | [3,7,12,16,20,21,25,29,30,38,46,47,51,55,60,64,68,69,73,77,78,86,94,95] |
| 4 | $\left[\frac{3}{4},\ \frac{3}{4},\ \frac{1}{4}\right]$ | [4,8,9,15,19,24,26,34,35,37,41,42,52,56,57,63,67,72,74,82,83,85,89,90] |

Table 4: Wyckoff site: 4d, site symmetry: 23.1'

| No. | position | mapping |
|---|---|---|
| 1 | $\left[\frac{3}{4},\ \frac{3}{4},\ \frac{3}{4}\right]$ | [1,5,6,14,22,23,27,31,36,40,44,45,49,53,54,62,70,71,75,79,84,88,92,93] |
| 2 | $\left[\frac{3}{4},\ \frac{1}{4},\ \frac{1}{4}\right]$ | [2,10,11,13,17,18,28,32,33,39,43,48,50,58,59,61,65,66,76,80,81,87,91,96] |
| 3 | $\left[\frac{1}{4},\ \frac{3}{4},\ \frac{1}{4}\right]$ | [3,7,12,16,20,21,25,29,30,38,46,47,51,55,60,64,68,69,73,77,78,86,94,95] |
| 4 | $\left[\frac{1}{4},\ \frac{1}{4},\ \frac{3}{4}\right]$ | [4,8,9,15,19,24,26,34,35,37,41,42,52,56,57,63,67,72,74,82,83,85,89,90] |

Table 5: Wyckoff site: 16e, site symmetry: .3.1'

| No. | position | mapping |
|---|---|---|
| 1 | $[x,\ x,\ x]$ | [1,5,6,49,53,54] |
| 2 | $[x,\ -x,\ -x]$ | [2,10,11,50,58,59] |

*continued ...*

Table 5

| No. | position | mapping |
|---|---|---|
| 3 | $[-x,\ x,\ -x]$ | [3,7,12,51,55,60] |
| 4 | $[-x,\ -x,\ x]$ | [4,8,9,52,56,57] |
| 5 | $\left[x,\ x+\frac{1}{2},\ x+\frac{1}{2}\right]$ | [13,17,18,61,65,66] |
| 6 | $\left[x,\ \frac{1}{2}-x,\ \frac{1}{2}-x\right]$ | [14,22,23,62,70,71] |
| 7 | $\left[-x,\ x+\frac{1}{2},\ \frac{1}{2}-x\right]$ | [15,19,24,63,67,72] |
| 8 | $\left[-x,\ \frac{1}{2}-x,\ x+\frac{1}{2}\right]$ | [16,20,21,64,68,69] |
| 9 | $\left[x+\frac{1}{2},\ x,\ x+\frac{1}{2}\right]$ | [25,29,30,73,77,78] |
| 10 | $\left[x+\frac{1}{2},\ -x,\ \frac{1}{2}-x\right]$ | [26,34,35,74,82,83] |
| 11 | $\left[\frac{1}{2}-x,\ x,\ \frac{1}{2}-x\right]$ | [27,31,36,75,79,84] |
| 12 | $\left[\frac{1}{2}-x,\ -x,\ x+\frac{1}{2}\right]$ | [28,32,33,76,80,81] |
| 13 | $\left[x+\frac{1}{2},\ x+\frac{1}{2},\ x\right]$ | [37,41,42,85,89,90] |
| 14 | $\left[x+\frac{1}{2},\ \frac{1}{2}-x,\ -x\right]$ | [38,46,47,86,94,95] |
| 15 | $\left[\frac{1}{2}-x,\ x+\frac{1}{2},\ -x\right]$ | [39,43,48,87,91,96] |
| 16 | $\left[\frac{1}{2}-x,\ \frac{1}{2}-x,\ x\right]$ | [40,44,45,88,92,93] |

Table 6: Wyckoff site: 24f, site symmetry: 2..1'

| No. | position | mapping |
|---|---|---|
| 1 | $[x,\ 0,\ 0]$ | [1,2,49,50] |
| 2 | $[-x,\ 0,\ 0]$ | [3,4,51,52] |
| 3 | $[0,\ x,\ 0]$ | [5,12,53,60] |
| 4 | $[0,\ 0,\ x]$ | [6,9,54,57] |
| 5 | $[0,\ 0,\ -x]$ | [7,11,55,59] |
| 6 | $[0,\ -x,\ 0]$ | [8,10,56,58] |
| 7 | $\left[x,\ \frac{1}{2},\ \frac{1}{2}\right]$ | [13,14,61,62] |
| 8 | $\left[-x,\ \frac{1}{2},\ \frac{1}{2}\right]$ | [15,16,63,64] |
| 9 | $\left[0,\ x+\frac{1}{2},\ \frac{1}{2}\right]$ | [17,24,65,72] |
| 10 | $\left[0,\ \frac{1}{2},\ x+\frac{1}{2}\right]$ | [18,21,66,69] |
| 11 | $\left[0,\ \frac{1}{2},\ \frac{1}{2}-x\right]$ | [19,23,67,71] |
| 12 | $\left[0,\ \frac{1}{2}-x,\ \frac{1}{2}\right]$ | [20,22,68,70] |
| 13 | $\left[x+\frac{1}{2},\ 0,\ \frac{1}{2}\right]$ | [25,26,73,74] |
| 14 | $\left[\frac{1}{2}-x,\ 0,\ \frac{1}{2}\right]$ | [27,28,75,76] |
| 15 | $\left[\frac{1}{2},\ x,\ \frac{1}{2}\right]$ | [29,36,77,84] |
| 16 | $\left[\frac{1}{2},\ 0,\ x+\frac{1}{2}\right]$ | [30,33,78,81] |
| 17 | $\left[\frac{1}{2},\ 0,\ \frac{1}{2}-x\right]$ | [31,35,79,83] |
| 18 | $\left[\frac{1}{2},\ -x,\ \frac{1}{2}\right]$ | [32,34,80,82] |
| 19 | $\left[x+\frac{1}{2},\ \frac{1}{2},\ 0\right]$ | [37,38,85,86] |
| 20 | $\left[\frac{1}{2}-x,\ \frac{1}{2},\ 0\right]$ | [39,40,87,88] |
| 21 | $\left[\frac{1}{2},\ x+\frac{1}{2},\ 0\right]$ | [41,48,89,96] |
| 22 | $\left[\frac{1}{2},\ \frac{1}{2},\ x\right]$ | [42,45,90,93] |
| 23 | $\left[\frac{1}{2},\ \frac{1}{2},\ -x\right]$ | [43,47,91,95] |
| 24 | $\left[\frac{1}{2},\ \frac{1}{2}-x,\ 0\right]$ | [44,46,92,94] |

Table 7: Wyckoff site: `24g`, site symmetry: `2..1'`

| No. | position | mapping |
|---|---|---|
| 1 | $\left[x,\ \frac{1}{4},\ \frac{1}{4}\right]$ | `[1,14,49,62]` |
| 2 | $\left[x,\ \frac{3}{4},\ \frac{3}{4}\right]$ | `[2,13,50,61]` |
| 3 | $\left[-x,\ \frac{1}{4},\ \frac{3}{4}\right]$ | `[3,16,51,64]` |
| 4 | $\left[-x,\ \frac{3}{4},\ \frac{1}{4}\right]$ | `[4,15,52,63]` |
| 5 | $\left[\frac{1}{4},\ x,\ \frac{1}{4}\right]$ | `[5,36,53,84]` |
| 6 | $\left[\frac{1}{4},\ \frac{1}{4},\ x\right]$ | `[6,45,54,93]` |
| 7 | $\left[\frac{3}{4},\ \frac{1}{4},\ -x\right]$ | `[7,47,55,95]` |
| 8 | $\left[\frac{3}{4},\ -x,\ \frac{1}{4}\right]$ | `[8,34,56,82]` |
| 9 | $\left[\frac{3}{4},\ \frac{3}{4},\ x\right]$ | `[9,42,57,90]` |
| 10 | $\left[\frac{1}{4},\ -x,\ \frac{3}{4}\right]$ | `[10,32,58,80]` |
| 11 | $\left[\frac{1}{4},\ \frac{3}{4},\ -x\right]$ | `[11,43,59,91]` |
| 12 | $\left[\frac{3}{4},\ x,\ \frac{3}{4}\right]$ | `[12,29,60,77]` |
| 13 | $\left[\frac{1}{4},\ x+\frac{1}{2},\ \frac{3}{4}\right]$ | `[17,48,65,96]` |
| 14 | $\left[\frac{1}{4},\ \frac{3}{4},\ x+\frac{1}{2}\right]$ | `[18,33,66,81]` |
| 15 | $\left[\frac{3}{4},\ \frac{3}{4},\ \frac{1}{2}-x\right]$ | `[19,35,67,83]` |
| 16 | $\left[\frac{3}{4},\ \frac{1}{2}-x,\ \frac{3}{4}\right]$ | `[20,46,68,94]` |
| 17 | $\left[\frac{3}{4},\ \frac{1}{4},\ x+\frac{1}{2}\right]$ | `[21,30,69,78]` |
| 18 | $\left[\frac{1}{4},\ \frac{1}{2}-x,\ \frac{1}{4}\right]$ | `[22,44,70,92]` |
| 19 | $\left[\frac{1}{4},\ \frac{1}{4},\ \frac{1}{2}-x\right]$ | `[23,31,71,79]` |
| 20 | $\left[\frac{3}{4},\ x+\frac{1}{2},\ \frac{1}{4}\right]$ | `[24,41,72,89]` |
| 21 | $\left[x+\frac{1}{2},\ \frac{1}{4},\ \frac{3}{4}\right]$ | `[25,38,73,86]` |
| 22 | $\left[x+\frac{1}{2},\ \frac{3}{4},\ \frac{1}{4}\right]$ | `[26,37,74,85]` |
| 23 | $\left[\frac{1}{2}-x,\ \frac{1}{4},\ \frac{1}{4}\right]$ | `[27,40,75,88]` |
| 24 | $\left[\frac{1}{2}-x,\ \frac{3}{4},\ \frac{3}{4}\right]$ | `[28,39,76,87]` |

Table 8: Wyckoff site: `48h`, site symmetry: `11'`

| No. | position | mapping |
|---|---|---|
| 1 | $[x,\ y,\ z]$ | `[1,49]` |
| 2 | $[x,\ -y,\ -z]$ | `[2,50]` |
| 3 | $[-x,\ y,\ -z]$ | `[3,51]` |
| 4 | $[-x,\ -y,\ z]$ | `[4,52]` |
| 5 | $[z,\ x,\ y]$ | `[5,53]` |
| 6 | $[y,\ z,\ x]$ | `[6,54]` |
| 7 | $[-y,\ z,\ -x]$ | `[7,55]` |
| 8 | $[-z,\ -x,\ y]$ | `[8,56]` |
| 9 | $[-y,\ -z,\ x]$ | `[9,57]` |
| 10 | $[z,\ -x,\ -y]$ | `[10,58]` |
| 11 | $[y,\ -z,\ -x]$ | `[11,59]` |
| 12 | $[-z,\ x,\ -y]$ | `[12,60]` |
| 13 | $\left[x,\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$ | `[13,61]` |
| 14 | $\left[x,\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$ | `[14,62]` |
| 15 | $\left[-x,\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$ | `[15,63]` |

*continued ...*

Table 8

| No. | position | mapping |
|---|---|---|
| 16 | $\left[-x,\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$ | [16,64] |
| 17 | $\left[z,\ x+\frac{1}{2},\ y+\frac{1}{2}\right]$ | [17,65] |
| 18 | $\left[y,\ z+\frac{1}{2},\ x+\frac{1}{2}\right]$ | [18,66] |
| 19 | $\left[-y,\ z+\frac{1}{2},\ \frac{1}{2}-x\right]$ | [19,67] |
| 20 | $\left[-z,\ \frac{1}{2}-x,\ y+\frac{1}{2}\right]$ | [20,68] |
| 21 | $\left[-y,\ \frac{1}{2}-z,\ x+\frac{1}{2}\right]$ | [21,69] |
| 22 | $\left[z,\ \frac{1}{2}-x,\ \frac{1}{2}-y\right]$ | [22,70] |
| 23 | $\left[y,\ \frac{1}{2}-z,\ \frac{1}{2}-x\right]$ | [23,71] |
| 24 | $\left[-z,\ x+\frac{1}{2},\ \frac{1}{2}-y\right]$ | [24,72] |
| 25 | $\left[x+\frac{1}{2},\ y,\ z+\frac{1}{2}\right]$ | [25,73] |
| 26 | $\left[x+\frac{1}{2},\ -y,\ \frac{1}{2}-z\right]$ | [26,74] |
| 27 | $\left[\frac{1}{2}-x,\ y,\ \frac{1}{2}-z\right]$ | [27,75] |
| 28 | $\left[\frac{1}{2}-x,\ -y,\ z+\frac{1}{2}\right]$ | [28,76] |
| 29 | $\left[z+\frac{1}{2},\ x,\ y+\frac{1}{2}\right]$ | [29,77] |
| 30 | $\left[y+\frac{1}{2},\ z,\ x+\frac{1}{2}\right]$ | [30,78] |
| 31 | $\left[\frac{1}{2}-y,\ z,\ \frac{1}{2}-x\right]$ | [31,79] |
| 32 | $\left[\frac{1}{2}-z,\ -x,\ y+\frac{1}{2}\right]$ | [32,80] |
| 33 | $\left[\frac{1}{2}-y,\ -z,\ x+\frac{1}{2}\right]$ | [33,81] |
| 34 | $\left[z+\frac{1}{2},\ -x,\ \frac{1}{2}-y\right]$ | [34,82] |
| 35 | $\left[y+\frac{1}{2},\ -z,\ \frac{1}{2}-x\right]$ | [35,83] |
| 36 | $\left[\frac{1}{2}-z,\ x,\ \frac{1}{2}-y\right]$ | [36,84] |
| 37 | $\left[x+\frac{1}{2},\ y+\frac{1}{2},\ z\right]$ | [37,85] |
| 38 | $\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ -z\right]$ | [38,86] |
| 39 | $\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ -z\right]$ | [39,87] |
| 40 | $\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ z\right]$ | [40,88] |
| 41 | $\left[z+\frac{1}{2},\ x+\frac{1}{2},\ y\right]$ | [41,89] |
| 42 | $\left[y+\frac{1}{2},\ z+\frac{1}{2},\ x\right]$ | [42,90] |
| 43 | $\left[\frac{1}{2}-y,\ z+\frac{1}{2},\ -x\right]$ | [43,91] |
| 44 | $\left[\frac{1}{2}-z,\ \frac{1}{2}-x,\ y\right]$ | [44,92] |
| 45 | $\left[\frac{1}{2}-y,\ \frac{1}{2}-z,\ x\right]$ | [45,93] |
| 46 | $\left[z+\frac{1}{2},\ \frac{1}{2}-x,\ -y\right]$ | [46,94] |
| 47 | $\left[y+\frac{1}{2},\ \frac{1}{2}-z,\ -x\right]$ | [47,95] |
| 48 | $\left[\frac{1}{2}-z,\ x+\frac{1}{2},\ -y\right]$ | [48,96] |