# MSG No. 230.147 $Ia'\bar{3}'d$ [ Type III, cubic ]

Table 1: Wyckoff site: `16a`, site symmetry: `.-3'.`

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

Table 2: Wyckoff site: `16b`, site symmetry: `.32'`

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

Table 3: Wyckoff site: `24c`, site symmetry: `2.2'2'`

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

Table 4: Wyckoff site: `24d`, site symmetry: `-4..`

| No. | position | mapping |
|---|---|---|
| 1 | $\left[\frac{3}{8}, 0, \frac{1}{4}\right]$ | `[1,2,14,61]` |
| 2 | $\left[\frac{1}{8}, 0, \frac{3}{4}\right]$ | `[3,52,69,70]` |
| 3 | $\left[\frac{5}{8}, \frac{1}{2}, \frac{1}{4}\right]$ | `[4,21,22,51]` |
| 4 | $\left[\frac{1}{4}, \frac{3}{8}, 0\right]$ | `[5,12,17,67]` |
| 5 | $\left[0, \frac{1}{4}, \frac{3}{8}\right]$ | `[6,9,23,64]` |
| 6 | $\left[\frac{1}{2}, \frac{1}{4}, \frac{5}{8}\right]$ | `[7,15,24,59]` |
| 7 | $\left[\frac{3}{4}, \frac{1}{8}, 0\right]$ | `[8,58,66,68]` |
| 8 | $\left[\frac{1}{4}, \frac{5}{8}, \frac{1}{2}\right]$ | `[10,18,20,56]` |
| 9 | $\left[0, \frac{3}{4}, \frac{1}{8}\right]$ | `[11,55,63,72]` |
| 10 | $\left[\frac{7}{8}, \frac{1}{2}, \frac{3}{4}\right]$ | `[13,49,50,62]` |
| 11 | $\left[\frac{1}{2}, \frac{3}{4}, \frac{7}{8}\right]$ | `[16,54,57,71]` |
| 12 | $\left[\frac{3}{4}, \frac{7}{8}, \frac{1}{2}\right]$ | `[19,53,60,65]` |
| 13 | $\left[\frac{5}{8}, 0, \frac{3}{4}\right]$ | `[25,37,38,74]` |
| 14 | $\left[\frac{1}{8}, \frac{1}{2}, \frac{1}{4}\right]$ | `[26,73,85,86]` |
| 15 | $\left[0, \frac{1}{4}, \frac{7}{8}\right]$ | `[27,36,47,91]` |

*continued ...*

Table 4

| No. | position | mapping |
|---|---|---|
| 16 | $\left[0,\ \frac{3}{4},\ \frac{5}{8}\right]$ | [28,42,45,83] |
| 17 | $\left[\frac{1}{4},\ \frac{1}{8},\ \frac{1}{2}\right]$ | [29,79,89,96] |
| 18 | $\left[\frac{1}{4},\ \frac{7}{8},\ 0\right]$ | [30,32,44,94] |
| 19 | $\left[\frac{3}{4},\ \frac{5}{8},\ 0\right]$ | [31,41,48,77] |
| 20 | $\left[\frac{7}{8},\ 0,\ \frac{1}{4}\right]$ | [33,34,39,88] |
| 21 | $\left[\frac{1}{2},\ \frac{1}{4},\ \frac{1}{8}\right]$ | [35,76,90,93] |
| 22 | $\left[\frac{3}{8},\ \frac{1}{2},\ \frac{3}{4}\right]$ | [40,81,82,87] |
| 23 | $\left[\frac{1}{2},\ \frac{3}{4},\ \frac{3}{8}\right]$ | [43,75,84,95] |
| 24 | $\left[\frac{3}{4},\ \frac{3}{8},\ \frac{1}{2}\right]$ | [46,78,80,92] |

Table 5: Wyckoff site: 32e, site symmetry: .3.

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

*continued ...*

Table 5

| No. | position | mapping |
|---|---|---|
| 32 | $\left[x+\frac{1}{2},\, x,\, \frac{1}{2}-x\right]$ | [88,92,93] |

Table 6: Wyckoff site: 48f, site symmetry: 2..

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

*continued ...*

Table 6

| No. | position | mapping |
|---|---|---|
| 40 | $\left[0,\ \frac{3}{4},\ x+\frac{3}{4}\right]$ | [63,72] |
| 41 | $\left[\frac{3}{4},\ x+\frac{3}{4},\ 0\right]$ | [66,68] |
| 42 | $\left[x+\frac{3}{4},\ 0,\ \frac{3}{4}\right]$ | [69,70] |
| 43 | $\left[\frac{1}{2},\ \frac{3}{4},\ \frac{3}{4}-x\right]$ | [75,84] |
| 44 | $\left[\frac{3}{4},\ \frac{3}{4}-x,\ \frac{1}{2}\right]$ | [78,80] |
| 45 | $\left[\frac{3}{4}-x,\ \frac{1}{2},\ \frac{3}{4}\right]$ | [81,82] |
| 46 | $\left[\frac{1}{2}-x,\ \frac{1}{2},\ \frac{1}{4}\right]$ | [85,86] |
| 47 | $\left[\frac{1}{4},\ \frac{1}{2}-x,\ \frac{1}{2}\right]$ | [89,96] |
| 48 | $\left[\frac{1}{2},\ \frac{1}{4},\ \frac{1}{2}-x\right]$ | [90,93] |

Table 7: Wyckoff site: 48g, site symmetry: ..2'

| No. | position | mapping |
|---|---|---|
| 1 | $\left[\frac{1}{8},\ y,\ \frac{1}{4}-y\right]$ | [1,34] |
| 2 | $\left[\frac{1}{8},\ -y,\ y+\frac{1}{4}\right]$ | [2,33] |
| 3 | $\left[\frac{3}{8},\ y,\ y+\frac{3}{4}\right]$ | [3,25] |
| 4 | $\left[\frac{7}{8},\ \frac{1}{2}-y,\ \frac{1}{4}-y\right]$ | [4,26] |
| 5 | $\left[\frac{1}{4}-y,\ \frac{1}{8},\ y\right]$ | [5,32] |
| 6 | $\left[y,\ \frac{1}{4}-y,\ \frac{1}{8}\right]$ | [6,36] |
| 7 | $\left[\frac{1}{2}-y,\ \frac{1}{4}-y,\ \frac{7}{8}\right]$ | [7,35] |
| 8 | $\left[y+\frac{3}{4},\ \frac{3}{8},\ y\right]$ | [8,31] |
| 9 | $\left[-y,\ y+\frac{1}{4},\ \frac{1}{8}\right]$ | [9,27] |
| 10 | $\left[\frac{1}{4}-y,\ \frac{7}{8},\ \frac{1}{2}-y\right]$ | [10,29] |
| 11 | $\left[y,\ y+\frac{3}{4},\ \frac{3}{8}\right]$ | [11,28] |
| 12 | $\left[y+\frac{1}{4},\ \frac{1}{8},\ -y\right]$ | [12,30] |
| 13 | $\left[\frac{1}{8},\ \frac{1}{2}-y,\ \frac{3}{4}-y\right]$ | [13,87] |
| 14 | $\left[\frac{5}{8},\ y,\ y+\frac{1}{4}\right]$ | [14,88] |
| 15 | $\left[y+\frac{1}{2},\ \frac{1}{4}-y,\ \frac{3}{8}\right]$ | [15,93] |
| 16 | $\left[\frac{1}{2}-y,\ \frac{3}{4}-y,\ \frac{1}{8}\right]$ | [16,95] |
| 17 | $\left[y+\frac{1}{4},\ \frac{5}{8},\ y\right]$ | [17,94] |
| 18 | $\left[\frac{1}{4}-y,\ \frac{3}{8},\ y+\frac{1}{2}\right]$ | [18,96] |
| 19 | $\left[\frac{3}{4}-y,\ \frac{1}{8},\ \frac{1}{2}-y\right]$ | [19,92] |
| 20 | $\left[y+\frac{1}{4},\ \frac{3}{8},\ \frac{1}{2}-y\right]$ | [20,89] |
| 21 | $\left[\frac{3}{8},\ y+\frac{1}{2},\ \frac{1}{4}-y\right]$ | [21,86] |
| 22 | $\left[\frac{3}{8},\ \frac{1}{2}-y,\ y+\frac{1}{4}\right]$ | [22,85] |
| 23 | $\left[y,\ y+\frac{1}{4},\ \frac{5}{8}\right]$ | [23,91] |
| 24 | $\left[\frac{1}{2}-y,\ y+\frac{1}{4},\ \frac{3}{8}\right]$ | [24,90] |
| 25 | $\left[\frac{7}{8},\ -y,\ y+\frac{3}{4}\right]$ | [37,70] |
| 26 | $\left[\frac{7}{8},\ y,\ \frac{3}{4}-y\right]$ | [38,69] |
| 27 | $\left[\frac{5}{8},\ -y,\ \frac{1}{4}-y\right]$ | [39,61] |
| 28 | $\left[\frac{1}{8},\ y+\frac{1}{2},\ y+\frac{3}{4}\right]$ | [40,62] |
| 29 | $\left[y+\frac{3}{4},\ \frac{7}{8},\ -y\right]$ | [41,68] |
| 30 | $\left[-y,\ y+\frac{3}{4},\ \frac{7}{8}\right]$ | [42,72] |
| 31 | $\left[y+\frac{1}{2},\ y+\frac{3}{4},\ \frac{1}{8}\right]$ | [43,71] |

*continued ...*

Table 7

| No. | position | mapping |
|---|---|---|
| 32 | $\left[\frac{1}{4}-y,\ \frac{5}{8},\ -y\right]$ | [44,67] |
| 33 | $\left[y,\ \frac{3}{4}-y,\ \frac{7}{8}\right]$ | [45,63] |
| 34 | $\left[y+\frac{3}{4},\ \frac{1}{8},\ y+\frac{1}{2}\right]$ | [46,65] |
| 35 | $\left[-y,\ \frac{1}{4}-y,\ \frac{5}{8}\right]$ | [47,64] |
| 36 | $\left[\frac{3}{4}-y,\ \frac{7}{8},\ y\right]$ | [48,66] |
| 37 | $\left[\frac{5}{8},\ y+\frac{1}{2},\ \frac{3}{4}-y\right]$ | [49,82] |
| 38 | $\left[\frac{5}{8},\ \frac{1}{2}-y,\ y+\frac{3}{4}\right]$ | [50,81] |
| 39 | $\left[\frac{7}{8},\ y+\frac{1}{2},\ y+\frac{1}{4}\right]$ | [51,73] |
| 40 | $\left[\frac{3}{8},\ -y,\ \frac{3}{4}-y\right]$ | [52,74] |
| 41 | $\left[\frac{3}{4}-y,\ \frac{5}{8},\ y+\frac{1}{2}\right]$ | [53,80] |
| 42 | $\left[y+\frac{1}{2},\ \frac{3}{4}-y,\ \frac{5}{8}\right]$ | [54,84] |
| 43 | $\left[-y,\ \frac{3}{4}-y,\ \frac{3}{8}\right]$ | [55,83] |
| 44 | $\left[y+\frac{1}{4},\ \frac{7}{8},\ y+\frac{1}{2}\right]$ | [56,79] |
| 45 | $\left[\frac{1}{2}-y,\ y+\frac{3}{4},\ \frac{5}{8}\right]$ | [57,75] |
| 46 | $\left[\frac{3}{4}-y,\ \frac{3}{8},\ -y\right]$ | [58,77] |
| 47 | $\left[y+\frac{1}{2},\ y+\frac{1}{4},\ \frac{7}{8}\right]$ | [59,76] |
| 48 | $\left[y+\frac{3}{4},\ \frac{5}{8},\ \frac{1}{2}-y\right]$ | [60,78] |

Table 8: Wyckoff site: 96h, site symmetry: 1

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

*continued ...*

Table 8

| No. | position | mapping |
|---|---|---|
| 24 | $\left[z+\frac{1}{4},\, y+\frac{1}{4},\, x+\frac{1}{4}\right]$ | [24] |
| 25 | $\left[x+\frac{1}{4},\, \frac{1}{4}-z,\, y+\frac{3}{4}\right]$ | [25] |
| 26 | $\left[x+\frac{3}{4},\, z+\frac{1}{4},\, \frac{1}{4}-y\right]$ | [26] |
| 27 | $\left[z+\frac{3}{4},\, y+\frac{1}{4},\, \frac{1}{4}-x\right]$ | [27] |
| 28 | $\left[\frac{1}{4}-z,\, y+\frac{3}{4},\, x+\frac{1}{4}\right]$ | [28] |
| 29 | $\left[\frac{1}{4}-y,\, x+\frac{3}{4},\, z+\frac{1}{4}\right]$ | [29] |
| 30 | $\left[y+\frac{1}{4},\, \frac{1}{4}-x,\, z+\frac{3}{4}\right]$ | [30] |
| 31 | $\left[y+\frac{3}{4},\, x+\frac{1}{4},\, \frac{1}{4}-z\right]$ | [31] |
| 32 | $\left[\frac{1}{4}-y,\, \frac{1}{4}-x,\, \frac{1}{4}-z\right]$ | [32] |
| 33 | $\left[\frac{1}{4}-x,\, z+\frac{3}{4},\, y+\frac{1}{4}\right]$ | [33] |
| 34 | $\left[\frac{1}{4}-x,\, \frac{1}{4}-z,\, \frac{1}{4}-y\right]$ | [34] |
| 35 | $\left[z+\frac{1}{4},\, \frac{1}{4}-y,\, x+\frac{3}{4}\right]$ | [35] |
| 36 | $\left[\frac{1}{4}-z,\, \frac{1}{4}-y,\, \frac{1}{4}-x\right]$ | [36] |
| 37 | $[-x,\, -y,\, -z]$ | [37] |
| 38 | $\left[-x,\, y,\, z+\frac{1}{2}\right]$ | [38] |
| 39 | $\left[x+\frac{1}{2},\, -y,\, z\right]$ | [39] |
| 40 | $\left[x,\, y+\frac{1}{2},\, -z\right]$ | [40] |
| 41 | $[-z,\, -x,\, -y]$ | [41] |
| 42 | $[-y,\, -z,\, -x]$ | [42] |
| 43 | $\left[y+\frac{1}{2},\, -z,\, x\right]$ | [43] |
| 44 | $\left[z,\, x+\frac{1}{2},\, -y\right]$ | [44] |
| 45 | $\left[y,\, z+\frac{1}{2},\, -x\right]$ | [45] |
| 46 | $\left[-z,\, x,\, y+\frac{1}{2}\right]$ | [46] |
| 47 | $\left[-y,\, z,\, x+\frac{1}{2}\right]$ | [47] |
| 48 | $\left[z+\frac{1}{2},\, -x,\, y\right]$ | [48] |
| 49 | $\left[x+\frac{1}{2},\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$ | [49] |
| 50 | $\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, -z\right]$ | [50] |
| 51 | $\left[-x,\, y+\frac{1}{2},\, \frac{1}{2}-z\right]$ | [51] |
| 52 | $\left[\frac{1}{2}-x,\, -y,\, z+\frac{1}{2}\right]$ | [52] |
| 53 | $\left[z+\frac{1}{2},\, x+\frac{1}{2},\, y+\frac{1}{2}\right]$ | [53] |
| 54 | $\left[y+\frac{1}{2},\, z+\frac{1}{2},\, x+\frac{1}{2}\right]$ | [54] |
| 55 | $\left[-y,\, z+\frac{1}{2},\, \frac{1}{2}-x\right]$ | [55] |
| 56 | $\left[\frac{1}{2}-z,\, -x,\, y+\frac{1}{2}\right]$ | [56] |
| 57 | $\left[\frac{1}{2}-y,\, -z,\, x+\frac{1}{2}\right]$ | [57] |
| 58 | $\left[z+\frac{1}{2},\, \frac{1}{2}-x,\, -y\right]$ | [58] |
| 59 | $\left[y+\frac{1}{2},\, \frac{1}{2}-z,\, -x\right]$ | [59] |
| 60 | $\left[-z,\, x+\frac{1}{2},\, \frac{1}{2}-y\right]$ | [60] |
| 61 | $\left[\frac{3}{4}-x,\, z+\frac{3}{4},\, \frac{1}{4}-y\right]$ | [61] |
| 62 | $\left[\frac{1}{4}-x,\, \frac{3}{4}-z,\, y+\frac{3}{4}\right]$ | [62] |
| 63 | $\left[\frac{1}{4}-z,\, \frac{3}{4}-y,\, x+\frac{3}{4}\right]$ | [63] |
| 64 | $\left[z+\frac{3}{4},\, \frac{1}{4}-y,\, \frac{3}{4}-x\right]$ | [64] |
| 65 | $\left[y+\frac{3}{4},\, \frac{1}{4}-x,\, \frac{3}{4}-z\right]$ | [65] |
| 66 | $\left[\frac{3}{4}-y,\, x+\frac{3}{4},\, \frac{1}{4}-z\right]$ | [66] |
| 67 | $\left[\frac{1}{4}-y,\, \frac{3}{4}-x,\, z+\frac{3}{4}\right]$ | [67] |
| 68 | $\left[y+\frac{3}{4},\, x+\frac{3}{4},\, z+\frac{3}{4}\right]$ | [68] |
| 69 | $\left[x+\frac{3}{4},\, \frac{1}{4}-z,\, \frac{3}{4}-y\right]$ | [69] |
| 70 | $\left[x+\frac{3}{4},\, z+\frac{3}{4},\, y+\frac{3}{4}\right]$ | [70] |

*continued ...*

Table 8

| No. | position | mapping |
|---|---|---|
| 71 | $\left[\frac{3}{4}-z,\, y+\frac{3}{4},\, \frac{1}{4}-x\right]$ | [71] |
| 72 | $\left[z+\frac{3}{4},\, y+\frac{3}{4},\, x+\frac{3}{4}\right]$ | [72] |
| 73 | $\left[x+\frac{3}{4},\, \frac{3}{4}-z,\, y+\frac{1}{4}\right]$ | [73] |
| 74 | $\left[x+\frac{1}{4},\, z+\frac{3}{4},\, \frac{3}{4}-y\right]$ | [74] |
| 75 | $\left[z+\frac{1}{4},\, y+\frac{3}{4},\, \frac{3}{4}-x\right]$ | [75] |
| 76 | $\left[\frac{3}{4}-z,\, y+\frac{1}{4},\, x+\frac{3}{4}\right]$ | [76] |
| 77 | $\left[\frac{3}{4}-y,\, x+\frac{1}{4},\, z+\frac{3}{4}\right]$ | [77] |
| 78 | $\left[y+\frac{3}{4},\, \frac{3}{4}-x,\, z+\frac{1}{4}\right]$ | [78] |
| 79 | $\left[y+\frac{1}{4},\, x+\frac{3}{4},\, \frac{3}{4}-z\right]$ | [79] |
| 80 | $\left[\frac{3}{4}-y,\, \frac{3}{4}-x,\, \frac{3}{4}-z\right]$ | [80] |
| 81 | $\left[\frac{3}{4}-x,\, z+\frac{1}{4},\, y+\frac{3}{4}\right]$ | [81] |
| 82 | $\left[\frac{3}{4}-x,\, \frac{3}{4}-z,\, \frac{3}{4}-y\right]$ | [82] |
| 83 | $\left[z+\frac{3}{4},\, \frac{3}{4}-y,\, x+\frac{1}{4}\right]$ | [83] |
| 84 | $\left[\frac{3}{4}-z,\, \frac{3}{4}-y,\, \frac{3}{4}-x\right]$ | [84] |
| 85 | $\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, \frac{1}{2}-z\right]$ | [85] |
| 86 | $\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, z\right]$ | [86] |
| 87 | $\left[x,\, \frac{1}{2}-y,\, z+\frac{1}{2}\right]$ | [87] |
| 88 | $\left[x+\frac{1}{2},\, y,\, \frac{1}{2}-z\right]$ | [88] |
| 89 | $\left[\frac{1}{2}-z,\, \frac{1}{2}-x,\, \frac{1}{2}-y\right]$ | [89] |
| 90 | $\left[\frac{1}{2}-y,\, \frac{1}{2}-z,\, \frac{1}{2}-x\right]$ | [90] |
| 91 | $\left[y,\, \frac{1}{2}-z,\, x+\frac{1}{2}\right]$ | [91] |
| 92 | $\left[z+\frac{1}{2},\, x,\, \frac{1}{2}-y\right]$ | [92] |
| 93 | $\left[y+\frac{1}{2},\, z,\, \frac{1}{2}-x\right]$ | [93] |
| 94 | $\left[\frac{1}{2}-z,\, x+\frac{1}{2},\, y\right]$ | [94] |
| 95 | $\left[\frac{1}{2}-y,\, z+\frac{1}{2},\, x\right]$ | [95] |
| 96 | $\left[z,\, \frac{1}{2}-x,\, y+\frac{1}{2}\right]$ | [96] |