

MSG No. 225.119  $Fm\bar{3}m'$  [ Type III, cubic ]

Table 1: Wyckoff site: 4a, site symmetry:  $m\bar{3}m'$

| 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]  |
| 2   | $[0, \frac{1}{2}, \frac{1}{2}]$ | [49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96]   |
| 3   | $[\frac{1}{2}, 0, \frac{1}{2}]$ | [97, 98, 99, 100, 101, 102, 103, 104, 105, 106, 107, 108, 109, 110, 111, 112, 113, 114, 115, 116, 117, 118, 119, 120, 121, 122, 123, 124, 125, 126, 127, 128, 129, 130, 131, 132, 133, 134, 135, 136, 137, 138, 139, 140, 141, 142, 143, 144]    |
| 4   | $[\frac{1}{2}, \frac{1}{2}, 0]$ | [145, 146, 147, 148, 149, 150, 151, 152, 153, 154, 155, 156, 157, 158, 159, 160, 161, 162, 163, 164, 165, 166, 167, 168, 169, 170, 171, 172, 173, 174, 175, 176, 177, 178, 179, 180, 181, 182, 183, 184, 185, 186, 187, 188, 189, 190, 191, 192] |

Table 2: Wyckoff site: 4b, site symmetry:  $m\bar{3}m'$

| No. | position                                  | mapping  |
|-----|---|--|
| 1   | $[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$ | [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]  |
| 2   | $[\frac{1}{2}, 0, 0]$                     | [49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96]   |
| 3   | $[0, \frac{1}{2}, 0]$                     | [97, 98, 99, 100, 101, 102, 103, 104, 105, 106, 107, 108, 109, 110, 111, 112, 113, 114, 115, 116, 117, 118, 119, 120, 121, 122, 123, 124, 125, 126, 127, 128, 129, 130, 131, 132, 133, 134, 135, 136, 137, 138, 139, 140, 141, 142, 143, 144]    |
| 4   | $[0, 0, \frac{1}{2}]$                     | [145, 146, 147, 148, 149, 150, 151, 152, 153, 154, 155, 156, 157, 158, 159, 160, 161, 162, 163, 164, 165, 166, 167, 168, 169, 170, 171, 172, 173, 174, 175, 176, 177, 178, 179, 180, 181, 182, 183, 184, 185, 186, 187, 188, 189, 190, 191, 192] |

Table 3: Wyckoff site: 8c, site symmetry:  $\bar{4}3m'$

| No. | position                                  | mapping  |
|-----|---|--|
| 1   | $[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$ | [1, 5, 6, 44, 46, 48, 50, 58, 59, 88, 89, 93, 99, 103, 108, 133, 138, 143, 148, 152, 153, 182, 183, 187]     |
| 2   | $[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$ | [2, 10, 11, 40, 41, 45, 49, 53, 54, 92, 94, 96, 100, 104, 105, 134, 135, 139, 147, 151, 156, 181, 186, 191]  |
| 3   | $[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$ | [3, 7, 12, 37, 42, 47, 52, 56, 57, 86, 87, 91, 97, 101, 102, 140, 142, 144, 146, 154, 155, 184, 185, 189]    |
| 4   | $[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}]$ | [4, 8, 9, 38, 39, 43, 51, 55, 60, 85, 90, 95, 98, 106, 107, 136, 137, 141, 145, 149, 150, 188, 190, 192]     |
| 5   | $[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$ | [13, 17, 18, 32, 34, 36, 62, 70, 71, 76, 77, 81, 111, 115, 120, 121, 126, 131, 160, 164, 165, 170, 171, 175] |
| 6   | $[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$ | [14, 22, 23, 28, 29, 33, 61, 65, 66, 80, 82, 84, 112, 116, 117, 122, 123, 127, 159, 163, 168, 169, 174, 179] |
| 7   | $[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$ | [15, 19, 24, 25, 30, 35, 64, 68, 69, 74, 75, 79, 109, 113, 114, 128, 130, 132, 158, 166, 167, 172, 173, 177] |
| 8   | $[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}]$ | [16, 20, 21, 26, 27, 31, 63, 67, 72, 73, 78, 83, 110, 118, 119, 124, 125, 129, 157, 161, 162, 176, 178, 180] |

Table 4: Wyckoff site: 24d, site symmetry:  $m.m'm'$ 

| No. | position                                  | mapping                                    |
|-----|---|--|
| 1   | $[0, \frac{1}{4}, \frac{1}{4}]$           | $[1, 14, 33, 46, 50, 61, 82, 93]$          |
| 2   | $[0, \frac{3}{4}, \frac{3}{4}]$           | $[2, 13, 34, 45, 49, 62, 81, 94]$          |
| 3   | $[0, \frac{1}{4}, \frac{3}{4}]$           | $[3, 16, 26, 37, 52, 63, 73, 86]$          |
| 4   | $[0, \frac{3}{4}, \frac{1}{4}]$           | $[4, 15, 25, 38, 51, 64, 74, 85]$          |
| 5   | $[\frac{1}{4}, 0, \frac{1}{4}]$           | $[5, 24, 30, 44, 108, 113, 128, 138]$      |
| 6   | $[\frac{1}{4}, \frac{1}{4}, 0]$           | $[6, 21, 27, 48, 153, 162, 180, 183]$      |
| 7   | $[\frac{3}{4}, \frac{1}{4}, 0]$           | $[7, 23, 28, 47, 155, 163, 179, 184]$      |
| 8   | $[\frac{3}{4}, 0, \frac{1}{4}]$           | $[8, 22, 29, 43, 106, 116, 127, 137]$      |
| 9   | $[\frac{3}{4}, \frac{3}{4}, 0]$           | $[9, 18, 36, 39, 150, 165, 171, 192]$      |
| 10  | $[\frac{1}{4}, 0, \frac{3}{4}]$           | $[10, 20, 31, 41, 104, 118, 125, 139]$     |
| 11  | $[\frac{1}{4}, \frac{3}{4}, 0]$           | $[11, 19, 35, 40, 151, 167, 172, 191]$     |
| 12  | $[\frac{3}{4}, 0, \frac{3}{4}]$           | $[12, 17, 32, 42, 101, 120, 126, 140]$     |
| 13  | $[\frac{1}{4}, \frac{1}{2}, \frac{3}{4}]$ | $[53, 72, 78, 92, 156, 161, 176, 186]$     |
| 14  | $[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}]$ | $[54, 69, 75, 96, 105, 114, 132, 135]$     |
| 15  | $[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}]$ | $[55, 71, 76, 95, 107, 115, 131, 136]$     |
| 16  | $[\frac{3}{4}, \frac{1}{2}, \frac{3}{4}]$ | $[56, 70, 77, 91, 154, 164, 175, 185]$     |
| 17  | $[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}]$ | $[57, 66, 84, 87, 102, 117, 123, 144]$     |
| 18  | $[\frac{1}{4}, \frac{1}{2}, \frac{1}{4}]$ | $[58, 68, 79, 89, 152, 166, 173, 187]$     |
| 19  | $[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}]$ | $[59, 67, 83, 88, 103, 119, 124, 143]$     |
| 20  | $[\frac{3}{4}, \frac{1}{2}, \frac{1}{4}]$ | $[60, 65, 80, 90, 149, 168, 174, 188]$     |
| 21  | $[\frac{1}{2}, \frac{1}{4}, \frac{3}{4}]$ | $[97, 110, 129, 142, 146, 157, 178, 189]$  |
| 22  | $[\frac{1}{2}, \frac{3}{4}, \frac{1}{4}]$ | $[98, 109, 130, 141, 145, 158, 177, 190]$  |
| 23  | $[\frac{1}{2}, \frac{1}{4}, \frac{1}{4}]$ | $[99, 112, 122, 133, 148, 159, 169, 182]$  |
| 24  | $[\frac{1}{2}, \frac{3}{4}, \frac{3}{4}]$ | $[100, 111, 121, 134, 147, 160, 170, 181]$ |

Table 5: Wyckoff site: 24e, site symmetry:  $4'm.m'$ 

| No. | position                            | mapping                                    |
|-----|-------------------------------------|--|
| 1   | $[x, 0, 0]$                         | $[1, 2, 15, 16, 25, 26, 45, 46]$           |
| 2   | $[-x, 0, 0]$                        | $[3, 4, 13, 14, 33, 34, 37, 38]$           |
| 3   | $[0, x, 0]$                         | $[5, 12, 20, 22, 29, 31, 42, 44]$          |
| 4   | $[0, 0, x]$                         | $[6, 9, 19, 23, 28, 35, 39, 48]$           |
| 5   | $[0, 0, -x]$                        | $[7, 11, 18, 21, 27, 36, 40, 47]$          |
| 6   | $[0, -x, 0]$                        | $[8, 10, 17, 24, 30, 32, 41, 43]$          |
| 7   | $[x, \frac{1}{2}, \frac{1}{2}]$     | $[49, 50, 63, 64, 73, 74, 93, 94]$         |
| 8   | $[-x, \frac{1}{2}, \frac{1}{2}]$    | $[51, 52, 61, 62, 81, 82, 85, 86]$         |
| 9   | $[0, x + \frac{1}{2}, \frac{1}{2}]$ | $[53, 60, 68, 70, 77, 79, 90, 92]$         |
| 10  | $[0, \frac{1}{2}, x + \frac{1}{2}]$ | $[54, 57, 67, 71, 76, 83, 87, 96]$         |
| 11  | $[0, \frac{1}{2}, \frac{1}{2} - x]$ | $[55, 59, 66, 69, 75, 84, 88, 95]$         |
| 12  | $[0, \frac{1}{2} - x, \frac{1}{2}]$ | $[56, 58, 65, 72, 78, 80, 89, 91]$         |
| 13  | $[x + \frac{1}{2}, 0, \frac{1}{2}]$ | $[97, 98, 111, 112, 121, 122, 141, 142]$   |
| 14  | $[\frac{1}{2} - x, 0, \frac{1}{2}]$ | $[99, 100, 109, 110, 129, 130, 133, 134]$  |
| 15  | $[\frac{1}{2}, x, \frac{1}{2}]$     | $[101, 108, 116, 118, 125, 127, 138, 140]$ |

*continued ...*

Table 5

| No. | position                            | mapping                                  |
|-----|-------------------------------------|--|
| 16  | $[\frac{1}{2}, 0, x + \frac{1}{2}]$ | [102, 105, 115, 119, 124, 131, 135, 144] |
| 17  | $[\frac{1}{2}, 0, \frac{1}{2} - x]$ | [103, 107, 114, 117, 123, 132, 136, 143] |
| 18  | $[\frac{1}{2}, -x, \frac{1}{2}]$    | [104, 106, 113, 120, 126, 128, 137, 139] |
| 19  | $[x + \frac{1}{2}, \frac{1}{2}, 0]$ | [145, 146, 159, 160, 169, 170, 189, 190] |
| 20  | $[\frac{1}{2} - x, \frac{1}{2}, 0]$ | [147, 148, 157, 158, 177, 178, 181, 182] |
| 21  | $[\frac{1}{2}, x + \frac{1}{2}, 0]$ | [149, 156, 164, 166, 173, 175, 186, 188] |
| 22  | $[\frac{1}{2}, \frac{1}{2}, x]$     | [150, 153, 163, 167, 172, 179, 183, 192] |
| 23  | $[\frac{1}{2}, \frac{1}{2}, -x]$    | [151, 155, 162, 165, 171, 180, 184, 191] |
| 24  | $[\frac{1}{2}, \frac{1}{2} - x, 0]$ | [152, 154, 161, 168, 174, 176, 185, 187] |

Table 6: Wyckoff site: 32f, site symmetry:  $.3\bar{m}'$ 

| No. | position                                 | mapping                        |
|-----|--|--------------------------------|
| 1   | $[x, x, x]$                              | [1, 5, 6, 44, 46, 48]          |
| 2   | $[x, -x, -x]$                            | [2, 10, 11, 40, 41, 45]        |
| 3   | $[-x, x, -x]$                            | [3, 7, 12, 37, 42, 47]         |
| 4   | $[-x, -x, x]$                            | [4, 8, 9, 38, 39, 43]          |
| 5   | $[-x, -x, -x]$                           | [13, 17, 18, 32, 34, 36]       |
| 6   | $[-x, x, x]$                             | [14, 22, 23, 28, 29, 33]       |
| 7   | $[x, -x, x]$                             | [15, 19, 24, 25, 30, 35]       |
| 8   | $[x, x, -x]$                             | [16, 20, 21, 26, 27, 31]       |
| 9   | $[x, x + \frac{1}{2}, x + \frac{1}{2}]$  | [49, 53, 54, 92, 94, 96]       |
| 10  | $[x, \frac{1}{2} - x, \frac{1}{2} - x]$  | [50, 58, 59, 88, 89, 93]       |
| 11  | $[-x, x + \frac{1}{2}, \frac{1}{2} - x]$ | [51, 55, 60, 85, 90, 95]       |
| 12  | $[-x, \frac{1}{2} - x, x + \frac{1}{2}]$ | [52, 56, 57, 86, 87, 91]       |
| 13  | $[-x, \frac{1}{2} - x, \frac{1}{2} - x]$ | [61, 65, 66, 80, 82, 84]       |
| 14  | $[-x, x + \frac{1}{2}, x + \frac{1}{2}]$ | [62, 70, 71, 76, 77, 81]       |
| 15  | $[x, \frac{1}{2} - x, x + \frac{1}{2}]$  | [63, 67, 72, 73, 78, 83]       |
| 16  | $[x, x + \frac{1}{2}, \frac{1}{2} - x]$  | [64, 68, 69, 74, 75, 79]       |
| 17  | $[x + \frac{1}{2}, x, x + \frac{1}{2}]$  | [97, 101, 102, 140, 142, 144]  |
| 18  | $[x + \frac{1}{2}, -x, \frac{1}{2} - x]$ | [98, 106, 107, 136, 137, 141]  |
| 19  | $[\frac{1}{2} - x, x, \frac{1}{2} - x]$  | [99, 103, 108, 133, 138, 143]  |
| 20  | $[\frac{1}{2} - x, -x, x + \frac{1}{2}]$ | [100, 104, 105, 134, 135, 139] |
| 21  | $[\frac{1}{2} - x, -x, \frac{1}{2} - x]$ | [109, 113, 114, 128, 130, 132] |
| 22  | $[\frac{1}{2} - x, x, x + \frac{1}{2}]$  | [110, 118, 119, 124, 125, 129] |
| 23  | $[x + \frac{1}{2}, -x, x + \frac{1}{2}]$ | [111, 115, 120, 121, 126, 131] |
| 24  | $[x + \frac{1}{2}, x, \frac{1}{2} - x]$  | [112, 116, 117, 122, 123, 127] |
| 25  | $[x + \frac{1}{2}, x + \frac{1}{2}, x]$  | [145, 149, 150, 188, 190, 192] |
| 26  | $[x + \frac{1}{2}, \frac{1}{2} - x, -x]$ | [146, 154, 155, 184, 185, 189] |
| 27  | $[\frac{1}{2} - x, x + \frac{1}{2}, -x]$ | [147, 151, 156, 181, 186, 191] |
| 28  | $[\frac{1}{2} - x, \frac{1}{2} - x, x]$  | [148, 152, 153, 182, 183, 187] |
| 29  | $[\frac{1}{2} - x, \frac{1}{2} - x, -x]$ | [157, 161, 162, 176, 178, 180] |
| 30  | $[\frac{1}{2} - x, x + \frac{1}{2}, x]$  | [158, 166, 167, 172, 173, 177] |
| 31  | $[x + \frac{1}{2}, \frac{1}{2} - x, x]$  | [159, 163, 168, 169, 174, 179] |

*continued ...*

Table 6

| No. | position                                 | mapping                        |
|-----|--|--------------------------------|
| 32  | $[x + \frac{1}{2}, x + \frac{1}{2}, -x]$ | [160, 164, 165, 170, 171, 175] |

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

| No. | position                                      | mapping            |
|-----|---|--------------------|
| 1   | $[x, \frac{1}{4}, \frac{1}{4}]$               | [1, 46, 50, 93]    |
| 2   | $[x, \frac{3}{4}, \frac{3}{4}]$               | [2, 45, 49, 94]    |
| 3   | $[-x, \frac{1}{4}, \frac{3}{4}]$              | [3, 37, 52, 86]    |
| 4   | $[-x, \frac{3}{4}, \frac{1}{4}]$              | [4, 38, 51, 85]    |
| 5   | $[\frac{1}{4}, x, \frac{1}{4}]$               | [5, 44, 108, 138]  |
| 6   | $[\frac{1}{4}, \frac{1}{4}, x]$               | [6, 48, 153, 183]  |
| 7   | $[\frac{3}{4}, \frac{1}{4}, -x]$              | [7, 47, 155, 184]  |
| 8   | $[\frac{3}{4}, -x, \frac{1}{4}]$              | [8, 43, 106, 137]  |
| 9   | $[\frac{3}{4}, \frac{3}{4}, x]$               | [9, 39, 150, 192]  |
| 10  | $[\frac{1}{4}, -x, \frac{3}{4}]$              | [10, 41, 104, 139] |
| 11  | $[\frac{1}{4}, \frac{3}{4}, -x]$              | [11, 40, 151, 191] |
| 12  | $[\frac{3}{4}, x, \frac{3}{4}]$               | [12, 42, 101, 140] |
| 13  | $[-x, \frac{3}{4}, \frac{3}{4}]$              | [13, 34, 62, 81]   |
| 14  | $[-x, \frac{1}{4}, \frac{1}{4}]$              | [14, 33, 61, 82]   |
| 15  | $[x, \frac{3}{4}, \frac{1}{4}]$               | [15, 25, 64, 74]   |
| 16  | $[x, \frac{1}{4}, \frac{3}{4}]$               | [16, 26, 63, 73]   |
| 17  | $[\frac{3}{4}, -x, \frac{3}{4}]$              | [17, 32, 120, 126] |
| 18  | $[\frac{3}{4}, \frac{3}{4}, -x]$              | [18, 36, 165, 171] |
| 19  | $[\frac{1}{4}, \frac{3}{4}, x]$               | [19, 35, 167, 172] |
| 20  | $[\frac{1}{4}, x, \frac{3}{4}]$               | [20, 31, 118, 125] |
| 21  | $[\frac{1}{4}, \frac{1}{4}, -x]$              | [21, 27, 162, 180] |
| 22  | $[\frac{3}{4}, x, \frac{1}{4}]$               | [22, 29, 116, 127] |
| 23  | $[\frac{3}{4}, \frac{1}{4}, x]$               | [23, 28, 163, 179] |
| 24  | $[\frac{1}{4}, -x, \frac{1}{4}]$              | [24, 30, 113, 128] |
| 25  | $[\frac{1}{4}, x + \frac{1}{2}, \frac{3}{4}]$ | [53, 92, 156, 186] |
| 26  | $[\frac{1}{4}, \frac{3}{4}, x + \frac{1}{2}]$ | [54, 96, 105, 135] |
| 27  | $[\frac{3}{4}, \frac{3}{4}, \frac{1}{2} - x]$ | [55, 95, 107, 136] |
| 28  | $[\frac{3}{4}, \frac{1}{2} - x, \frac{3}{4}]$ | [56, 91, 154, 185] |
| 29  | $[\frac{3}{4}, \frac{1}{4}, x + \frac{1}{2}]$ | [57, 87, 102, 144] |
| 30  | $[\frac{1}{4}, \frac{1}{2} - x, \frac{1}{4}]$ | [58, 89, 152, 187] |
| 31  | $[\frac{1}{4}, \frac{1}{4}, \frac{1}{2} - x]$ | [59, 88, 103, 143] |
| 32  | $[\frac{3}{4}, x + \frac{1}{2}, \frac{1}{4}]$ | [60, 90, 149, 188] |
| 33  | $[\frac{3}{4}, \frac{1}{2} - x, \frac{1}{4}]$ | [65, 80, 168, 174] |
| 34  | $[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - x]$ | [66, 84, 117, 123] |
| 35  | $[\frac{1}{4}, \frac{1}{4}, x + \frac{1}{2}]$ | [67, 83, 119, 124] |
| 36  | $[\frac{1}{4}, x + \frac{1}{2}, \frac{1}{4}]$ | [68, 79, 166, 173] |
| 37  | $[\frac{1}{4}, \frac{3}{4}, \frac{1}{2} - x]$ | [69, 75, 114, 132] |
| 38  | $[\frac{3}{4}, x + \frac{1}{2}, \frac{3}{4}]$ | [70, 77, 164, 175] |
| 39  | $[\frac{3}{4}, \frac{3}{4}, x + \frac{1}{2}]$ | [71, 76, 115, 131] |

*continued ...*

Table 7

| No. | position                                      | mapping              |
|-----|---|----------------------|
| 40  | $[\frac{1}{4}, \frac{1}{2} - x, \frac{3}{4}]$ | [72, 78, 161, 176]   |
| 41  | $[x + \frac{1}{2}, \frac{1}{4}, \frac{3}{4}]$ | [97, 142, 146, 189]  |
| 42  | $[x + \frac{1}{2}, \frac{3}{4}, \frac{1}{4}]$ | [98, 141, 145, 190]  |
| 43  | $[\frac{1}{2} - x, \frac{1}{4}, \frac{1}{4}]$ | [99, 133, 148, 182]  |
| 44  | $[\frac{1}{2} - x, \frac{3}{4}, \frac{3}{4}]$ | [100, 134, 147, 181] |
| 45  | $[\frac{1}{2} - x, \frac{3}{4}, \frac{1}{4}]$ | [109, 130, 158, 177] |
| 46  | $[\frac{1}{2} - x, \frac{1}{4}, \frac{3}{4}]$ | [110, 129, 157, 178] |
| 47  | $[x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}]$ | [111, 121, 160, 170] |
| 48  | $[x + \frac{1}{2}, \frac{1}{4}, \frac{1}{4}]$ | [112, 122, 159, 169] |

Table 8: Wyckoff site: 48h, site symmetry:  $m.2'm'$ 

| No. | position                                | mapping              |
|-----|---|----------------------|
| 1   | $[0, y, y]$                             | [1, 14, 33, 46]      |
| 2   | $[0, -y, -y]$                           | [2, 13, 34, 45]      |
| 3   | $[0, y, -y]$                            | [3, 16, 26, 37]      |
| 4   | $[0, -y, y]$                            | [4, 15, 25, 38]      |
| 5   | $[y, 0, y]$                             | [5, 24, 30, 44]      |
| 6   | $[y, y, 0]$                             | [6, 21, 27, 48]      |
| 7   | $[-y, y, 0]$                            | [7, 23, 28, 47]      |
| 8   | $[-y, 0, y]$                            | [8, 22, 29, 43]      |
| 9   | $[-y, -y, 0]$                           | [9, 18, 36, 39]      |
| 10  | $[y, 0, -y]$                            | [10, 20, 31, 41]     |
| 11  | $[y, -y, 0]$                            | [11, 19, 35, 40]     |
| 12  | $[-y, 0, -y]$                           | [12, 17, 32, 42]     |
| 13  | $[0, y + \frac{1}{2}, y + \frac{1}{2}]$ | [49, 62, 81, 94]     |
| 14  | $[0, \frac{1}{2} - y, \frac{1}{2} - y]$ | [50, 61, 82, 93]     |
| 15  | $[0, y + \frac{1}{2}, \frac{1}{2} - y]$ | [51, 64, 74, 85]     |
| 16  | $[0, \frac{1}{2} - y, y + \frac{1}{2}]$ | [52, 63, 73, 86]     |
| 17  | $[y, \frac{1}{2}, y + \frac{1}{2}]$     | [53, 72, 78, 92]     |
| 18  | $[y, y + \frac{1}{2}, \frac{1}{2}]$     | [54, 69, 75, 96]     |
| 19  | $[-y, y + \frac{1}{2}, \frac{1}{2}]$    | [55, 71, 76, 95]     |
| 20  | $[-y, \frac{1}{2}, y + \frac{1}{2}]$    | [56, 70, 77, 91]     |
| 21  | $[-y, \frac{1}{2} - y, \frac{1}{2}]$    | [57, 66, 84, 87]     |
| 22  | $[y, \frac{1}{2}, \frac{1}{2} - y]$     | [58, 68, 79, 89]     |
| 23  | $[y, \frac{1}{2} - y, \frac{1}{2}]$     | [59, 67, 83, 88]     |
| 24  | $[-y, \frac{1}{2}, \frac{1}{2} - y]$    | [60, 65, 80, 90]     |
| 25  | $[\frac{1}{2}, y, y + \frac{1}{2}]$     | [97, 110, 129, 142]  |
| 26  | $[\frac{1}{2}, -y, \frac{1}{2} - y]$    | [98, 109, 130, 141]  |
| 27  | $[\frac{1}{2}, y, \frac{1}{2} - y]$     | [99, 112, 122, 133]  |
| 28  | $[\frac{1}{2}, -y, y + \frac{1}{2}]$    | [100, 111, 121, 134] |
| 29  | $[y + \frac{1}{2}, 0, y + \frac{1}{2}]$ | [101, 120, 126, 140] |
| 30  | $[y + \frac{1}{2}, y, \frac{1}{2}]$     | [102, 117, 123, 144] |
| 31  | $[\frac{1}{2} - y, y, \frac{1}{2}]$     | [103, 119, 124, 143] |

continued ...

Table 8

| No. | position                                | mapping              |
|-----|---|----------------------|
| 32  | $[\frac{1}{2} - y, 0, y + \frac{1}{2}]$ | [104, 118, 125, 139] |
| 33  | $[\frac{1}{2} - y, -y, \frac{1}{2}]$    | [105, 114, 132, 135] |
| 34  | $[y + \frac{1}{2}, 0, \frac{1}{2} - y]$ | [106, 116, 127, 137] |
| 35  | $[y + \frac{1}{2}, -y, \frac{1}{2}]$    | [107, 115, 131, 136] |
| 36  | $[\frac{1}{2} - y, 0, \frac{1}{2} - y]$ | [108, 113, 128, 138] |
| 37  | $[\frac{1}{2}, y + \frac{1}{2}, y]$     | [145, 158, 177, 190] |
| 38  | $[\frac{1}{2}, \frac{1}{2} - y, -y]$    | [146, 157, 178, 189] |
| 39  | $[\frac{1}{2}, y + \frac{1}{2}, -y]$    | [147, 160, 170, 181] |
| 40  | $[\frac{1}{2}, \frac{1}{2} - y, y]$     | [148, 159, 169, 182] |
| 41  | $[y + \frac{1}{2}, \frac{1}{2}, y]$     | [149, 168, 174, 188] |
| 42  | $[y + \frac{1}{2}, y + \frac{1}{2}, 0]$ | [150, 165, 171, 192] |
| 43  | $[\frac{1}{2} - y, y + \frac{1}{2}, 0]$ | [151, 167, 172, 191] |
| 44  | $[\frac{1}{2} - y, \frac{1}{2}, y]$     | [152, 166, 173, 187] |
| 45  | $[\frac{1}{2} - y, \frac{1}{2} - y, 0]$ | [153, 162, 180, 183] |
| 46  | $[y + \frac{1}{2}, \frac{1}{2}, -y]$    | [154, 164, 175, 185] |
| 47  | $[y + \frac{1}{2}, \frac{1}{2} - y, 0]$ | [155, 163, 179, 184] |
| 48  | $[\frac{1}{2} - y, \frac{1}{2}, -y]$    | [156, 161, 176, 186] |

Table 9: Wyckoff site: 48i, site symmetry:  $m.2'm'$ 

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

continued ...

Table 9

| No. | position  | mapping              |
|-----|---|----------------------|
| 24  | $[-y, 0, \frac{1}{2} - y]$                        | [60, 65, 80, 90]     |
| 25  | $[0, y, y + \frac{1}{2}]$                         | [97, 110, 129, 142]  |
| 26  | $[0, -y, \frac{1}{2} - y]$                        | [98, 109, 130, 141]  |
| 27  | $[0, y, \frac{1}{2} - y]$                         | [99, 112, 122, 133]  |
| 28  | $[0, -y, y + \frac{1}{2}]$                        | [100, 111, 121, 134] |
| 29  | $[y + \frac{1}{2}, \frac{1}{2}, y + \frac{1}{2}]$ | [101, 120, 126, 140] |
| 30  | $[y + \frac{1}{2}, y, 0]$                         | [102, 117, 123, 144] |
| 31  | $[\frac{1}{2} - y, y, 0]$                         | [103, 119, 124, 143] |
| 32  | $[\frac{1}{2} - y, \frac{1}{2}, y + \frac{1}{2}]$ | [104, 118, 125, 139] |
| 33  | $[\frac{1}{2} - y, -y, 0]$                        | [105, 114, 132, 135] |
| 34  | $[y + \frac{1}{2}, \frac{1}{2}, \frac{1}{2} - y]$ | [106, 116, 127, 137] |
| 35  | $[y + \frac{1}{2}, -y, 0]$                        | [107, 115, 131, 136] |
| 36  | $[\frac{1}{2} - y, \frac{1}{2}, \frac{1}{2} - y]$ | [108, 113, 128, 138] |
| 37  | $[0, y + \frac{1}{2}, y]$                         | [145, 158, 177, 190] |
| 38  | $[0, \frac{1}{2} - y, -y]$                        | [146, 157, 178, 189] |
| 39  | $[0, y + \frac{1}{2}, -y]$                        | [147, 160, 170, 181] |
| 40  | $[0, \frac{1}{2} - y, y]$                         | [148, 159, 169, 182] |
| 41  | $[y + \frac{1}{2}, 0, y]$                         | [149, 168, 174, 188] |
| 42  | $[y + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}]$ | [150, 165, 171, 192] |
| 43  | $[\frac{1}{2} - y, y + \frac{1}{2}, \frac{1}{2}]$ | [151, 167, 172, 191] |
| 44  | $[\frac{1}{2} - y, 0, y]$                         | [152, 166, 173, 187] |
| 45  | $[\frac{1}{2} - y, \frac{1}{2} - y, \frac{1}{2}]$ | [153, 162, 180, 183] |
| 46  | $[y + \frac{1}{2}, 0, -y]$                        | [154, 164, 175, 185] |
| 47  | $[y + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}]$ | [155, 163, 179, 184] |
| 48  | $[\frac{1}{2} - y, 0, -y]$                        | [156, 161, 176, 186] |

Table 10: Wyckoff site: 96j, site symmetry:  $m..$ 

| No. | position      | mapping  |
|-----|---------------|----------|
| 1   | $[0, y, z]$   | [1, 14]  |
| 2   | $[0, -y, -z]$ | [2, 13]  |
| 3   | $[0, y, -z]$  | [3, 16]  |
| 4   | $[0, -y, z]$  | [4, 15]  |
| 5   | $[z, 0, y]$   | [5, 24]  |
| 6   | $[y, z, 0]$   | [6, 21]  |
| 7   | $[-y, z, 0]$  | [7, 23]  |
| 8   | $[-z, 0, y]$  | [8, 22]  |
| 9   | $[-y, -z, 0]$ | [9, 18]  |
| 10  | $[z, 0, -y]$  | [10, 20] |
| 11  | $[y, -z, 0]$  | [11, 19] |
| 12  | $[-z, 0, -y]$ | [12, 17] |
| 13  | $[0, -z, y]$  | [25, 38] |
| 14  | $[0, z, -y]$  | [26, 37] |
| 15  | $[z, y, 0]$   | [27, 48] |

continued ...

Table 10

| No. | position                                | mapping    |
|-----|---|------------|
| 16  | $[-z, y, 0]$                            | [28, 47]   |
| 17  | $[-y, 0, z]$                            | [29, 43]   |
| 18  | $[y, 0, z]$                             | [30, 44]   |
| 19  | $[y, 0, -z]$                            | [31, 41]   |
| 20  | $[-y, 0, -z]$                           | [32, 42]   |
| 21  | $[0, z, y]$                             | [33, 46]   |
| 22  | $[0, -z, -y]$                           | [34, 45]   |
| 23  | $[z, -y, 0]$                            | [35, 40]   |
| 24  | $[-z, -y, 0]$                           | [36, 39]   |
| 25  | $[0, y + \frac{1}{2}, z + \frac{1}{2}]$ | [49, 62]   |
| 26  | $[0, \frac{1}{2} - y, \frac{1}{2} - z]$ | [50, 61]   |
| 27  | $[0, y + \frac{1}{2}, \frac{1}{2} - z]$ | [51, 64]   |
| 28  | $[0, \frac{1}{2} - y, z + \frac{1}{2}]$ | [52, 63]   |
| 29  | $[z, \frac{1}{2}, y + \frac{1}{2}]$     | [53, 72]   |
| 30  | $[y, z + \frac{1}{2}, \frac{1}{2}]$     | [54, 69]   |
| 31  | $[-y, z + \frac{1}{2}, \frac{1}{2}]$    | [55, 71]   |
| 32  | $[-z, \frac{1}{2}, y + \frac{1}{2}]$    | [56, 70]   |
| 33  | $[-y, \frac{1}{2} - z, \frac{1}{2}]$    | [57, 66]   |
| 34  | $[z, \frac{1}{2}, \frac{1}{2} - y]$     | [58, 68]   |
| 35  | $[y, \frac{1}{2} - z, \frac{1}{2}]$     | [59, 67]   |
| 36  | $[-z, \frac{1}{2}, \frac{1}{2} - y]$    | [60, 65]   |
| 37  | $[0, \frac{1}{2} - z, y + \frac{1}{2}]$ | [73, 86]   |
| 38  | $[0, z + \frac{1}{2}, \frac{1}{2} - y]$ | [74, 85]   |
| 39  | $[z, y + \frac{1}{2}, \frac{1}{2}]$     | [75, 96]   |
| 40  | $[-z, y + \frac{1}{2}, \frac{1}{2}]$    | [76, 95]   |
| 41  | $[-y, \frac{1}{2}, z + \frac{1}{2}]$    | [77, 91]   |
| 42  | $[y, \frac{1}{2}, z + \frac{1}{2}]$     | [78, 92]   |
| 43  | $[y, \frac{1}{2}, \frac{1}{2} - z]$     | [79, 89]   |
| 44  | $[-y, \frac{1}{2}, \frac{1}{2} - z]$    | [80, 90]   |
| 45  | $[0, z + \frac{1}{2}, y + \frac{1}{2}]$ | [81, 94]   |
| 46  | $[0, \frac{1}{2} - z, \frac{1}{2} - y]$ | [82, 93]   |
| 47  | $[z, \frac{1}{2} - y, \frac{1}{2}]$     | [83, 88]   |
| 48  | $[-z, \frac{1}{2} - y, \frac{1}{2}]$    | [84, 87]   |
| 49  | $[\frac{1}{2}, y, z + \frac{1}{2}]$     | [97, 110]  |
| 50  | $[\frac{1}{2}, -y, \frac{1}{2} - z]$    | [98, 109]  |
| 51  | $[\frac{1}{2}, y, \frac{1}{2} - z]$     | [99, 112]  |
| 52  | $[\frac{1}{2}, -y, z + \frac{1}{2}]$    | [100, 111] |
| 53  | $[z + \frac{1}{2}, 0, y + \frac{1}{2}]$ | [101, 120] |
| 54  | $[y + \frac{1}{2}, z, \frac{1}{2}]$     | [102, 117] |
| 55  | $[\frac{1}{2} - y, z, \frac{1}{2}]$     | [103, 119] |
| 56  | $[\frac{1}{2} - z, 0, y + \frac{1}{2}]$ | [104, 118] |
| 57  | $[\frac{1}{2} - y, -z, \frac{1}{2}]$    | [105, 114] |
| 58  | $[z + \frac{1}{2}, 0, \frac{1}{2} - y]$ | [106, 116] |
| 59  | $[y + \frac{1}{2}, -z, \frac{1}{2}]$    | [107, 115] |
| 60  | $[\frac{1}{2} - z, 0, \frac{1}{2} - y]$ | [108, 113] |
| 61  | $[\frac{1}{2}, -z, y + \frac{1}{2}]$    | [121, 134] |
| 62  | $[\frac{1}{2}, z, \frac{1}{2} - y]$     | [122, 133] |

continued ...



Table 10

| No. | position                                | mapping    |
|-----|---|------------|
| 63  | $[z + \frac{1}{2}, y, \frac{1}{2}]$     | [123, 144] |
| 64  | $[\frac{1}{2} - z, y, \frac{1}{2}]$     | [124, 143] |
| 65  | $[\frac{1}{2} - y, 0, z + \frac{1}{2}]$ | [125, 139] |
| 66  | $[y + \frac{1}{2}, 0, z + \frac{1}{2}]$ | [126, 140] |
| 67  | $[y + \frac{1}{2}, 0, \frac{1}{2} - z]$ | [127, 137] |
| 68  | $[\frac{1}{2} - y, 0, \frac{1}{2} - z]$ | [128, 138] |
| 69  | $[\frac{1}{2}, z, y + \frac{1}{2}]$     | [129, 142] |
| 70  | $[\frac{1}{2}, -z, \frac{1}{2} - y]$    | [130, 141] |
| 71  | $[z + \frac{1}{2}, -y, \frac{1}{2}]$    | [131, 136] |
| 72  | $[\frac{1}{2} - z, -y, \frac{1}{2}]$    | [132, 135] |
| 73  | $[\frac{1}{2}, y + \frac{1}{2}, z]$     | [145, 158] |
| 74  | $[\frac{1}{2}, \frac{1}{2} - y, -z]$    | [146, 157] |
| 75  | $[\frac{1}{2}, y + \frac{1}{2}, -z]$    | [147, 160] |
| 76  | $[\frac{1}{2}, \frac{1}{2} - y, z]$     | [148, 159] |
| 77  | $[z + \frac{1}{2}, \frac{1}{2}, y]$     | [149, 168] |
| 78  | $[y + \frac{1}{2}, z + \frac{1}{2}, 0]$ | [150, 165] |
| 79  | $[\frac{1}{2} - y, z + \frac{1}{2}, 0]$ | [151, 167] |
| 80  | $[\frac{1}{2} - z, \frac{1}{2}, y]$     | [152, 166] |
| 81  | $[\frac{1}{2} - y, \frac{1}{2} - z, 0]$ | [153, 162] |
| 82  | $[z + \frac{1}{2}, \frac{1}{2}, -y]$    | [154, 164] |
| 83  | $[y + \frac{1}{2}, \frac{1}{2} - z, 0]$ | [155, 163] |
| 84  | $[\frac{1}{2} - z, \frac{1}{2}, -y]$    | [156, 161] |
| 85  | $[\frac{1}{2}, \frac{1}{2} - z, y]$     | [169, 182] |
| 86  | $[\frac{1}{2}, z + \frac{1}{2}, -y]$    | [170, 181] |
| 87  | $[z + \frac{1}{2}, y + \frac{1}{2}, 0]$ | [171, 192] |
| 88  | $[\frac{1}{2} - z, y + \frac{1}{2}, 0]$ | [172, 191] |
| 89  | $[\frac{1}{2} - y, \frac{1}{2}, z]$     | [173, 187] |
| 90  | $[y + \frac{1}{2}, \frac{1}{2}, z]$     | [174, 188] |
| 91  | $[y + \frac{1}{2}, \frac{1}{2}, -z]$    | [175, 185] |
| 92  | $[\frac{1}{2} - y, \frac{1}{2}, -z]$    | [176, 186] |
| 93  | $[\frac{1}{2}, z + \frac{1}{2}, y]$     | [177, 190] |
| 94  | $[\frac{1}{2}, \frac{1}{2} - z, -y]$    | [178, 189] |
| 95  | $[z + \frac{1}{2}, \frac{1}{2} - y, 0]$ | [179, 184] |
| 96  | $[\frac{1}{2} - z, \frac{1}{2} - y, 0]$ | [180, 183] |

Table 11: Wyckoff site: 96k, site symmetry:  $\bar{3}m'$ 

| No. | position      | mapping |
|-----|---------------|---------|
| 1   | $[x, x, z]$   | [1, 44] |
| 2   | $[x, -x, -z]$ | [2, 41] |
| 3   | $[-x, x, -z]$ | [3, 42] |
| 4   | $[-x, -x, z]$ | [4, 43] |
| 5   | $[z, x, x]$   | [5, 48] |
| 6   | $[x, z, x]$   | [6, 46] |

*continued ...*

Table 11

| No. | position                                 | mapping   |
|-----|--|-----------|
| 7   | $[-x, z, -x]$                            | [7,37]    |
| 8   | $[-z, -x, x]$                            | [8,39]    |
| 9   | $[-x, -z, x]$                            | [9,38]    |
| 10  | $[z, -x, -x]$                            | [10,40]   |
| 11  | $[x, -z, -x]$                            | [11,45]   |
| 12  | $[-z, x, -x]$                            | [12,47]   |
| 13  | $[-x, -x, -z]$                           | [13,32]   |
| 14  | $[-x, x, z]$                             | [14,29]   |
| 15  | $[x, -x, z]$                             | [15,30]   |
| 16  | $[x, x, -z]$                             | [16,31]   |
| 17  | $[-z, -x, -x]$                           | [17,36]   |
| 18  | $[-x, -z, -x]$                           | [18,34]   |
| 19  | $[x, -z, x]$                             | [19,25]   |
| 20  | $[z, x, -x]$                             | [20,27]   |
| 21  | $[x, z, -x]$                             | [21,26]   |
| 22  | $[-z, x, x]$                             | [22,28]   |
| 23  | $[-x, z, x]$                             | [23,33]   |
| 24  | $[z, -x, x]$                             | [24,35]   |
| 25  | $[x, x + \frac{1}{2}, z + \frac{1}{2}]$  | [49,92]   |
| 26  | $[x, \frac{1}{2} - x, \frac{1}{2} - z]$  | [50,89]   |
| 27  | $[-x, x + \frac{1}{2}, \frac{1}{2} - z]$ | [51,90]   |
| 28  | $[-x, \frac{1}{2} - x, z + \frac{1}{2}]$ | [52,91]   |
| 29  | $[z, x + \frac{1}{2}, x + \frac{1}{2}]$  | [53,96]   |
| 30  | $[x, z + \frac{1}{2}, x + \frac{1}{2}]$  | [54,94]   |
| 31  | $[-x, z + \frac{1}{2}, \frac{1}{2} - x]$ | [55,85]   |
| 32  | $[-z, \frac{1}{2} - x, x + \frac{1}{2}]$ | [56,87]   |
| 33  | $[-x, \frac{1}{2} - z, x + \frac{1}{2}]$ | [57,86]   |
| 34  | $[z, \frac{1}{2} - x, \frac{1}{2} - x]$  | [58,88]   |
| 35  | $[x, \frac{1}{2} - z, \frac{1}{2} - x]$  | [59,93]   |
| 36  | $[-z, x + \frac{1}{2}, \frac{1}{2} - x]$ | [60,95]   |
| 37  | $[-x, \frac{1}{2} - x, \frac{1}{2} - z]$ | [61,80]   |
| 38  | $[-x, x + \frac{1}{2}, z + \frac{1}{2}]$ | [62,77]   |
| 39  | $[x, \frac{1}{2} - x, z + \frac{1}{2}]$  | [63,78]   |
| 40  | $[x, x + \frac{1}{2}, \frac{1}{2} - z]$  | [64,79]   |
| 41  | $[-z, \frac{1}{2} - x, \frac{1}{2} - x]$ | [65,84]   |
| 42  | $[-x, \frac{1}{2} - z, \frac{1}{2} - x]$ | [66,82]   |
| 43  | $[x, \frac{1}{2} - z, x + \frac{1}{2}]$  | [67,73]   |
| 44  | $[z, x + \frac{1}{2}, \frac{1}{2} - x]$  | [68,75]   |
| 45  | $[x, z + \frac{1}{2}, \frac{1}{2} - x]$  | [69,74]   |
| 46  | $[-z, x + \frac{1}{2}, x + \frac{1}{2}]$ | [70,76]   |
| 47  | $[-x, z + \frac{1}{2}, x + \frac{1}{2}]$ | [71,81]   |
| 48  | $[z, \frac{1}{2} - x, x + \frac{1}{2}]$  | [72,83]   |
| 49  | $[x + \frac{1}{2}, x, z + \frac{1}{2}]$  | [97,140]  |
| 50  | $[x + \frac{1}{2}, -x, \frac{1}{2} - z]$ | [98,137]  |
| 51  | $[\frac{1}{2} - x, x, \frac{1}{2} - z]$  | [99,138]  |
| 52  | $[\frac{1}{2} - x, -x, z + \frac{1}{2}]$ | [100,139] |
| 53  | $[z + \frac{1}{2}, x, x + \frac{1}{2}]$  | [101,144] |

continued ...

Table 11

| No. | position                                 | mapping   |
|-----|--|-----------|
| 54  | $[x + \frac{1}{2}, z, x + \frac{1}{2}]$  | [102,142] |
| 55  | $[\frac{1}{2} - x, z, \frac{1}{2} - x]$  | [103,133] |
| 56  | $[\frac{1}{2} - z, -x, x + \frac{1}{2}]$ | [104,135] |
| 57  | $[\frac{1}{2} - x, -z, x + \frac{1}{2}]$ | [105,134] |
| 58  | $[z + \frac{1}{2}, -x, \frac{1}{2} - x]$ | [106,136] |
| 59  | $[x + \frac{1}{2}, -z, \frac{1}{2} - x]$ | [107,141] |
| 60  | $[\frac{1}{2} - z, x, \frac{1}{2} - x]$  | [108,143] |
| 61  | $[\frac{1}{2} - x, -x, \frac{1}{2} - z]$ | [109,128] |
| 62  | $[\frac{1}{2} - x, x, z + \frac{1}{2}]$  | [110,125] |
| 63  | $[x + \frac{1}{2}, -x, z + \frac{1}{2}]$ | [111,126] |
| 64  | $[x + \frac{1}{2}, x, \frac{1}{2} - z]$  | [112,127] |
| 65  | $[\frac{1}{2} - z, -x, \frac{1}{2} - x]$ | [113,132] |
| 66  | $[\frac{1}{2} - x, -z, \frac{1}{2} - x]$ | [114,130] |
| 67  | $[x + \frac{1}{2}, -z, x + \frac{1}{2}]$ | [115,121] |
| 68  | $[z + \frac{1}{2}, x, \frac{1}{2} - x]$  | [116,123] |
| 69  | $[x + \frac{1}{2}, z, \frac{1}{2} - x]$  | [117,122] |
| 70  | $[\frac{1}{2} - z, x, x + \frac{1}{2}]$  | [118,124] |
| 71  | $[\frac{1}{2} - x, z, x + \frac{1}{2}]$  | [119,129] |
| 72  | $[z + \frac{1}{2}, -x, x + \frac{1}{2}]$ | [120,131] |
| 73  | $[x + \frac{1}{2}, x + \frac{1}{2}, z]$  | [145,188] |
| 74  | $[x + \frac{1}{2}, \frac{1}{2} - x, -z]$ | [146,185] |
| 75  | $[\frac{1}{2} - x, x + \frac{1}{2}, -z]$ | [147,186] |
| 76  | $[\frac{1}{2} - x, \frac{1}{2} - x, z]$  | [148,187] |
| 77  | $[z + \frac{1}{2}, x + \frac{1}{2}, x]$  | [149,192] |
| 78  | $[x + \frac{1}{2}, z + \frac{1}{2}, x]$  | [150,190] |
| 79  | $[\frac{1}{2} - x, z + \frac{1}{2}, -x]$ | [151,181] |
| 80  | $[\frac{1}{2} - z, \frac{1}{2} - x, x]$  | [152,183] |
| 81  | $[\frac{1}{2} - x, \frac{1}{2} - z, x]$  | [153,182] |
| 82  | $[z + \frac{1}{2}, \frac{1}{2} - x, -x]$ | [154,184] |
| 83  | $[x + \frac{1}{2}, \frac{1}{2} - z, -x]$ | [155,189] |
| 84  | $[\frac{1}{2} - z, x + \frac{1}{2}, -x]$ | [156,191] |
| 85  | $[\frac{1}{2} - x, \frac{1}{2} - x, -z]$ | [157,176] |
| 86  | $[\frac{1}{2} - x, x + \frac{1}{2}, z]$  | [158,173] |
| 87  | $[x + \frac{1}{2}, \frac{1}{2} - x, z]$  | [159,174] |
| 88  | $[x + \frac{1}{2}, x + \frac{1}{2}, -z]$ | [160,175] |
| 89  | $[\frac{1}{2} - z, \frac{1}{2} - x, -x]$ | [161,180] |
| 90  | $[\frac{1}{2} - x, \frac{1}{2} - z, -x]$ | [162,178] |
| 91  | $[x + \frac{1}{2}, \frac{1}{2} - z, x]$  | [163,169] |
| 92  | $[z + \frac{1}{2}, x + \frac{1}{2}, -x]$ | [164,171] |
| 93  | $[x + \frac{1}{2}, z + \frac{1}{2}, -x]$ | [165,170] |
| 94  | $[\frac{1}{2} - z, x + \frac{1}{2}, x]$  | [166,172] |
| 95  | $[\frac{1}{2} - x, z + \frac{1}{2}, x]$  | [167,177] |
| 96  | $[z + \frac{1}{2}, \frac{1}{2} - x, x]$  | [168,179] |

Table 12: Wyckoff site: 1921, 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  | $[-x, -y, -z]$ | [13]    |
| 14  | $[-x, y, z]$   | [14]    |
| 15  | $[x, -y, z]$   | [15]    |
| 16  | $[x, y, -z]$   | [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  | $[x, -z, y]$   | [25]    |
| 26  | $[x, z, -y]$   | [26]    |
| 27  | $[z, y, -x]$   | [27]    |
| 28  | $[-z, y, x]$   | [28]    |
| 29  | $[-y, x, z]$   | [29]    |
| 30  | $[y, -x, z]$   | [30]    |
| 31  | $[y, x, -z]$   | [31]    |
| 32  | $[-y, -x, -z]$ | [32]    |
| 33  | $[-x, z, y]$   | [33]    |
| 34  | $[-x, -z, -y]$ | [34]    |
| 35  | $[z, -y, x]$   | [35]    |
| 36  | $[-z, -y, -x]$ | [36]    |
| 37  | $[-x, z, -y]$  | [37]    |
| 38  | $[-x, -z, y]$  | [38]    |
| 39  | $[-z, -y, x]$  | [39]    |
| 40  | $[z, -y, -x]$  | [40]    |
| 41  | $[y, -x, -z]$  | [41]    |
| 42  | $[-y, x, -z]$  | [42]    |
| 43  | $[-y, -x, z]$  | [43]    |
| 44  | $[y, x, z]$    | [44]    |
| 45  | $[x, -z, -y]$  | [45]    |
| 46  | $[x, z, y]$    | [46]    |

*continued ...*

Table 12

| No. | position                                 | mapping |
|-----|--|---------|
| 47  | $[-z, y, -x]$                            | [47]    |
| 48  | $[z, y, x]$                              | [48]    |
| 49  | $[x, y + \frac{1}{2}, z + \frac{1}{2}]$  | [49]    |
| 50  | $[x, \frac{1}{2} - y, \frac{1}{2} - z]$  | [50]    |
| 51  | $[-x, y + \frac{1}{2}, \frac{1}{2} - z]$ | [51]    |
| 52  | $[-x, \frac{1}{2} - y, z + \frac{1}{2}]$ | [52]    |
| 53  | $[z, x + \frac{1}{2}, y + \frac{1}{2}]$  | [53]    |
| 54  | $[y, z + \frac{1}{2}, x + \frac{1}{2}]$  | [54]    |
| 55  | $[-y, z + \frac{1}{2}, \frac{1}{2} - x]$ | [55]    |
| 56  | $[-z, \frac{1}{2} - x, y + \frac{1}{2}]$ | [56]    |
| 57  | $[-y, \frac{1}{2} - z, x + \frac{1}{2}]$ | [57]    |
| 58  | $[z, \frac{1}{2} - x, \frac{1}{2} - y]$  | [58]    |
| 59  | $[y, \frac{1}{2} - z, \frac{1}{2} - x]$  | [59]    |
| 60  | $[-z, x + \frac{1}{2}, \frac{1}{2} - y]$ | [60]    |
| 61  | $[-x, \frac{1}{2} - y, \frac{1}{2} - z]$ | [61]    |
| 62  | $[-x, y + \frac{1}{2}, z + \frac{1}{2}]$ | [62]    |
| 63  | $[x, \frac{1}{2} - y, z + \frac{1}{2}]$  | [63]    |
| 64  | $[x, y + \frac{1}{2}, \frac{1}{2} - z]$  | [64]    |
| 65  | $[-z, \frac{1}{2} - x, \frac{1}{2} - y]$ | [65]    |
| 66  | $[-y, \frac{1}{2} - z, \frac{1}{2} - x]$ | [66]    |
| 67  | $[y, \frac{1}{2} - z, x + \frac{1}{2}]$  | [67]    |
| 68  | $[z, x + \frac{1}{2}, \frac{1}{2} - y]$  | [68]    |
| 69  | $[y, z + \frac{1}{2}, \frac{1}{2} - x]$  | [69]    |
| 70  | $[-z, x + \frac{1}{2}, y + \frac{1}{2}]$ | [70]    |
| 71  | $[-y, z + \frac{1}{2}, x + \frac{1}{2}]$ | [71]    |
| 72  | $[z, \frac{1}{2} - x, y + \frac{1}{2}]$  | [72]    |
| 73  | $[x, \frac{1}{2} - z, y + \frac{1}{2}]$  | [73]    |
| 74  | $[x, z + \frac{1}{2}, \frac{1}{2} - y]$  | [74]    |
| 75  | $[z, y + \frac{1}{2}, \frac{1}{2} - x]$  | [75]    |
| 76  | $[-z, y + \frac{1}{2}, x + \frac{1}{2}]$ | [76]    |
| 77  | $[-y, x + \frac{1}{2}, z + \frac{1}{2}]$ | [77]    |
| 78  | $[y, \frac{1}{2} - x, z + \frac{1}{2}]$  | [78]    |
| 79  | $[y, x + \frac{1}{2}, \frac{1}{2} - z]$  | [79]    |
| 80  | $[-y, \frac{1}{2} - x, \frac{1}{2} - z]$ | [80]    |
| 81  | $[-x, z + \frac{1}{2}, y + \frac{1}{2}]$ | [81]    |
| 82  | $[-x, \frac{1}{2} - z, \frac{1}{2} - y]$ | [82]    |
| 83  | $[z, \frac{1}{2} - y, x + \frac{1}{2}]$  | [83]    |
| 84  | $[-z, \frac{1}{2} - y, \frac{1}{2} - x]$ | [84]    |
| 85  | $[-x, z + \frac{1}{2}, \frac{1}{2} - y]$ | [85]    |
| 86  | $[-x, \frac{1}{2} - z, y + \frac{1}{2}]$ | [86]    |
| 87  | $[-z, \frac{1}{2} - y, x + \frac{1}{2}]$ | [87]    |
| 88  | $[z, \frac{1}{2} - y, \frac{1}{2} - x]$  | [88]    |
| 89  | $[y, \frac{1}{2} - x, \frac{1}{2} - z]$  | [89]    |
| 90  | $[-y, x + \frac{1}{2}, \frac{1}{2} - z]$ | [90]    |
| 91  | $[-y, \frac{1}{2} - x, z + \frac{1}{2}]$ | [91]    |
| 92  | $[y, x + \frac{1}{2}, z + \frac{1}{2}]$  | [92]    |
| 93  | $[x, \frac{1}{2} - z, \frac{1}{2} - y]$  | [93]    |

continued ...

Table 12

| No. | position                                 | mapping |
|-----|--|---------|
| 94  | $[x, z + \frac{1}{2}, y + \frac{1}{2}]$  | [94]    |
| 95  | $[-z, y + \frac{1}{2}, \frac{1}{2} - x]$ | [95]    |
| 96  | $[z, y + \frac{1}{2}, x + \frac{1}{2}]$  | [96]    |
| 97  | $[x + \frac{1}{2}, y, z + \frac{1}{2}]$  | [97]    |
| 98  | $[x + \frac{1}{2}, -y, \frac{1}{2} - z]$ | [98]    |
| 99  | $[\frac{1}{2} - x, y, \frac{1}{2} - z]$  | [99]    |
| 100 | $[\frac{1}{2} - x, -y, z + \frac{1}{2}]$ | [100]   |
| 101 | $[z + \frac{1}{2}, x, y + \frac{1}{2}]$  | [101]   |
| 102 | $[y + \frac{1}{2}, z, x + \frac{1}{2}]$  | [102]   |
| 103 | $[\frac{1}{2} - y, z, \frac{1}{2} - x]$  | [103]   |
| 104 | $[\frac{1}{2} - z, -x, y + \frac{1}{2}]$ | [104]   |
| 105 | $[\frac{1}{2} - y, -z, x + \frac{1}{2}]$ | [105]   |
| 106 | $[z + \frac{1}{2}, -x, \frac{1}{2} - y]$ | [106]   |
| 107 | $[y + \frac{1}{2}, -z, \frac{1}{2} - x]$ | [107]   |
| 108 | $[\frac{1}{2} - z, x, \frac{1}{2} - y]$  | [108]   |
| 109 | $[\frac{1}{2} - x, -y, \frac{1}{2} - z]$ | [109]   |
| 110 | $[\frac{1}{2} - x, y, z + \frac{1}{2}]$  | [110]   |
| 111 | $[x + \frac{1}{2}, -y, z + \frac{1}{2}]$ | [111]   |
| 112 | $[x + \frac{1}{2}, y, \frac{1}{2} - z]$  | [112]   |
| 113 | $[\frac{1}{2} - z, -x, \frac{1}{2} - y]$ | [113]   |
| 114 | $[\frac{1}{2} - y, -z, \frac{1}{2} - x]$ | [114]   |
| 115 | $[y + \frac{1}{2}, -z, x + \frac{1}{2}]$ | [115]   |
| 116 | $[z + \frac{1}{2}, x, \frac{1}{2} - y]$  | [116]   |
| 117 | $[y + \frac{1}{2}, z, \frac{1}{2} - x]$  | [117]   |
| 118 | $[\frac{1}{2} - z, x, y + \frac{1}{2}]$  | [118]   |
| 119 | $[\frac{1}{2} - y, z, x + \frac{1}{2}]$  | [119]   |
| 120 | $[z + \frac{1}{2}, -x, y + \frac{1}{2}]$ | [120]   |
| 121 | $[x + \frac{1}{2}, -z, y + \frac{1}{2}]$ | [121]   |
| 122 | $[x + \frac{1}{2}, z, \frac{1}{2} - y]$  | [122]   |
| 123 | $[z + \frac{1}{2}, y, \frac{1}{2} - x]$  | [123]   |
| 124 | $[\frac{1}{2} - z, y, x + \frac{1}{2}]$  | [124]   |
| 125 | $[\frac{1}{2} - y, x, z + \frac{1}{2}]$  | [125]   |
| 126 | $[y + \frac{1}{2}, -x, z + \frac{1}{2}]$ | [126]   |
| 127 | $[y + \frac{1}{2}, x, \frac{1}{2} - z]$  | [127]   |
| 128 | $[\frac{1}{2} - y, -x, \frac{1}{2} - z]$ | [128]   |
| 129 | $[\frac{1}{2} - x, z, y + \frac{1}{2}]$  | [129]   |
| 130 | $[\frac{1}{2} - x, -z, \frac{1}{2} - y]$ | [130]   |
| 131 | $[z + \frac{1}{2}, -y, x + \frac{1}{2}]$ | [131]   |
| 132 | $[\frac{1}{2} - z, -y, \frac{1}{2} - x]$ | [132]   |
| 133 | $[\frac{1}{2} - x, z, \frac{1}{2} - y]$  | [133]   |
| 134 | $[\frac{1}{2} - x, -z, y + \frac{1}{2}]$ | [134]   |
| 135 | $[\frac{1}{2} - z, -y, x + \frac{1}{2}]$ | [135]   |
| 136 | $[z + \frac{1}{2}, -y, \frac{1}{2} - x]$ | [136]   |
| 137 | $[y + \frac{1}{2}, -x, \frac{1}{2} - z]$ | [137]   |
| 138 | $[\frac{1}{2} - y, x, \frac{1}{2} - z]$  | [138]   |
| 139 | $[\frac{1}{2} - y, -x, z + \frac{1}{2}]$ | [139]   |
| 140 | $[y + \frac{1}{2}, x, z + \frac{1}{2}]$  | [140]   |

continued ...

Table 12

| No. | position                                 | mapping |
|-----|--|---------|
| 141 | $[x + \frac{1}{2}, -z, \frac{1}{2} - y]$ | [141]   |
| 142 | $[x + \frac{1}{2}, z, y + \frac{1}{2}]$  | [142]   |
| 143 | $[\frac{1}{2} - z, y, \frac{1}{2} - x]$  | [143]   |
| 144 | $[z + \frac{1}{2}, y, x + \frac{1}{2}]$  | [144]   |
| 145 | $[x + \frac{1}{2}, y + \frac{1}{2}, z]$  | [145]   |
| 146 | $[x + \frac{1}{2}, \frac{1}{2} - y, -z]$ | [146]   |
| 147 | $[\frac{1}{2} - x, y + \frac{1}{2}, -z]$ | [147]   |
| 148 | $[\frac{1}{2} - x, \frac{1}{2} - y, z]$  | [148]   |
| 149 | $[z + \frac{1}{2}, x + \frac{1}{2}, y]$  | [149]   |
| 150 | $[y + \frac{1}{2}, z + \frac{1}{2}, x]$  | [150]   |
| 151 | $[\frac{1}{2} - y, z + \frac{1}{2}, -x]$ | [151]   |
| 152 | $[\frac{1}{2} - z, \frac{1}{2} - x, y]$  | [152]   |
| 153 | $[\frac{1}{2} - y, \frac{1}{2} - z, x]$  | [153]   |
| 154 | $[z + \frac{1}{2}, \frac{1}{2} - x, -y]$ | [154]   |
| 155 | $[y + \frac{1}{2}, \frac{1}{2} - z, -x]$ | [155]   |
| 156 | $[\frac{1}{2} - z, x + \frac{1}{2}, -y]$ | [156]   |
| 157 | $[\frac{1}{2} - x, \frac{1}{2} - y, -z]$ | [157]   |
| 158 | $[\frac{1}{2} - x, y + \frac{1}{2}, z]$  | [158]   |
| 159 | $[x + \frac{1}{2}, \frac{1}{2} - y, z]$  | [159]   |
| 160 | $[x + \frac{1}{2}, y + \frac{1}{2}, -z]$ | [160]   |
| 161 | $[\frac{1}{2} - z, \frac{1}{2} - x, -y]$ | [161]   |
| 162 | $[\frac{1}{2} - y, \frac{1}{2} - z, -x]$ | [162]   |
| 163 | $[y + \frac{1}{2}, \frac{1}{2} - z, x]$  | [163]   |
| 164 | $[z + \frac{1}{2}, x + \frac{1}{2}, -y]$ | [164]   |
| 165 | $[y + \frac{1}{2}, z + \frac{1}{2}, -x]$ | [165]   |
| 166 | $[\frac{1}{2} - z, x + \frac{1}{2}, y]$  | [166]   |
| 167 | $[\frac{1}{2} - y, z + \frac{1}{2}, x]$  | [167]   |
| 168 | $[z + \frac{1}{2}, \frac{1}{2} - x, y]$  | [168]   |
| 169 | $[x + \frac{1}{2}, \frac{1}{2} - z, y]$  | [169]   |
| 170 | $[x + \frac{1}{2}, z + \frac{1}{2}, -y]$ | [170]   |
| 171 | $[z + \frac{1}{2}, y + \frac{1}{2}, -x]$ | [171]   |
| 172 | $[\frac{1}{2} - z, y + \frac{1}{2}, x]$  | [172]   |
| 173 | $[\frac{1}{2} - y, x + \frac{1}{2}, z]$  | [173]   |
| 174 | $[y + \frac{1}{2}, \frac{1}{2} - x, z]$  | [174]   |
| 175 | $[y + \frac{1}{2}, x + \frac{1}{2}, -z]$ | [175]   |
| 176 | $[\frac{1}{2} - y, \frac{1}{2} - x, -z]$ | [176]   |
| 177 | $[\frac{1}{2} - x, z + \frac{1}{2}, y]$  | [177]   |
| 178 | $[\frac{1}{2} - x, \frac{1}{2} - z, -y]$ | [178]   |
| 179 | $[z + \frac{1}{2}, \frac{1}{2} - y, x]$  | [179]   |
| 180 | $[\frac{1}{2} - z, \frac{1}{2} - y, -x]$ | [180]   |
| 181 | $[\frac{1}{2} - x, z + \frac{1}{2}, -y]$ | [181]   |
| 182 | $[\frac{1}{2} - x, \frac{1}{2} - z, y]$  | [182]   |
| 183 | $[\frac{1}{2} - z, \frac{1}{2} - y, x]$  | [183]   |
| 184 | $[z + \frac{1}{2}, \frac{1}{2} - y, -x]$ | [184]   |
| 185 | $[y + \frac{1}{2}, \frac{1}{2} - x, -z]$ | [185]   |
| 186 | $[\frac{1}{2} - y, x + \frac{1}{2}, -z]$ | [186]   |
| 187 | $[\frac{1}{2} - y, \frac{1}{2} - x, z]$  | [187]   |

continued ...

Table 12

| No. | position                                 | mapping |
|-----|--|---------|
| 188 | $[y + \frac{1}{2}, x + \frac{1}{2}, z]$  | [188]   |
| 189 | $[x + \frac{1}{2}, \frac{1}{2} - z, -y]$ | [189]   |
| 190 | $[x + \frac{1}{2}, z + \frac{1}{2}, y]$  | [190]   |
| 191 | $[\frac{1}{2} - z, y + \frac{1}{2}, -x]$ | [191]   |
| 192 | $[z + \frac{1}{2}, y + \frac{1}{2}, x]$  | [192]   |