

MSG No. 228.134 $Fd\bar{3}c$ [Type I, cubic]

Table 1: Wyckoff site: 16a, site symmetry: 23 .

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

Table 2: Wyckoff site: 32b, site symmetry: $\bar{3}2$

| No. | position | mapping |
|-----|-------------------------------------------|-----------------------------|
| 1 | $[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$ | [1, 12, 14, 16, 17, 18] |
| 2 | $[\frac{1}{2}, \frac{1}{4}, \frac{1}{2}]$ | [2, 7, 15, 105, 115, 120] |
| 3 | $[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$ | [3, 4, 11, 154, 164, 165] |
| 4 | $[\frac{1}{4}, \frac{1}{2}, \frac{1}{2}]$ | [5, 6, 13, 56, 70, 71] |
| 5 | $[\frac{1}{4}, 0, 0]$ | [8, 22, 23, 53, 54, 61] |
| 6 | $[0, \frac{1}{4}, 0]$ | [9, 19, 24, 98, 103, 111] |
| 7 | $[0, 0, \frac{1}{4}]$ | [10, 20, 21, 147, 148, 155] |
| 8 | $[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$ | [25, 36, 38, 40, 41, 42] |
| 9 | $[0, \frac{3}{4}, 0]$ | [26, 31, 39, 129, 139, 144] |
| 10 | $[0, 0, \frac{3}{4}]$ | [27, 28, 35, 178, 188, 189] |
| 11 | $[\frac{3}{4}, 0, 0]$ | [29, 30, 37, 80, 94, 95] |
| 12 | $[\frac{3}{4}, \frac{1}{2}, \frac{1}{2}]$ | [32, 46, 47, 77, 78, 85] |
| 13 | $[\frac{1}{2}, \frac{3}{4}, \frac{1}{2}]$ | [33, 43, 48, 122, 127, 135] |
| 14 | $[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$ | [34, 44, 45, 171, 172, 179] |
| 15 | $[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$ | [49, 60, 62, 64, 65, 66] |
| 16 | $[\frac{1}{2}, \frac{3}{4}, 0]$ | [50, 55, 63, 153, 163, 168] |
| 17 | $[\frac{1}{2}, 0, \frac{3}{4}]$ | [51, 52, 59, 106, 116, 117] |
| 18 | $[0, \frac{3}{4}, \frac{1}{2}]$ | [57, 67, 72, 146, 151, 159] |
| 19 | $[0, \frac{1}{2}, \frac{3}{4}]$ | [58, 68, 69, 99, 100, 107] |
| 20 | $[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$ | [73, 84, 86, 88, 89, 90] |
| 21 | $[0, \frac{1}{4}, \frac{1}{2}]$ | [74, 79, 87, 177, 187, 192] |

continued ...

Table 2

| No. | position | mapping |
|-----|-------------------------------------------|--------------------------------|
| 22 | $[0, \frac{1}{2}, \frac{1}{4}]$ | [75, 76, 83, 130, 140, 141] |
| 23 | $[\frac{1}{2}, \frac{1}{4}, 0]$ | [81, 91, 96, 170, 175, 183] |
| 24 | $[\frac{1}{2}, 0, \frac{1}{4}]$ | [82, 92, 93, 123, 124, 131] |
| 25 | $[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$ | [97, 108, 110, 112, 113, 114] |
| 26 | $[\frac{3}{4}, \frac{1}{2}, 0]$ | [101, 102, 109, 152, 166, 167] |
| 27 | $[\frac{3}{4}, 0, \frac{1}{2}]$ | [104, 118, 119, 149, 150, 157] |
| 28 | $[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$ | [121, 132, 134, 136, 137, 138] |
| 29 | $[\frac{1}{4}, 0, \frac{1}{2}]$ | [125, 126, 133, 176, 190, 191] |
| 30 | $[\frac{1}{4}, \frac{1}{2}, 0]$ | [128, 142, 143, 173, 174, 181] |
| 31 | $[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}]$ | [145, 156, 158, 160, 161, 162] |
| 32 | $[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}]$ | [169, 180, 182, 184, 185, 186] |

Table 3: Wyckoff site: $32c$, site symmetry: $.-3$.

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

continued ...

Table 3

| No. | position | mapping |
|-----|-------------------------------------------|--------------------------------|
| 30 | $[\frac{3}{4}, \frac{1}{2}, \frac{1}{4}]$ | [153, 163, 168, 177, 187, 192] |
| 31 | $[\frac{3}{4}, \frac{3}{4}, 0]$ | [154, 164, 165, 178, 188, 189] |
| 32 | $[0, 0, \frac{1}{2}]$ | [156, 158, 160, 180, 182, 184] |

Table 4: Wyckoff site: 48d, site symmetry: $-4..$

| No. | position | mapping |
|-----|-------------------------------------------|---------------------|
| 1 | $[\frac{7}{8}, \frac{1}{8}, \frac{1}{8}]$ | [1, 8, 123, 170] |
| 2 | $[\frac{1}{8}, \frac{3}{8}, \frac{3}{8}]$ | [2, 3, 32, 73] |
| 3 | $[\frac{3}{8}, \frac{3}{8}, \frac{5}{8}]$ | [4, 16, 91, 143] |
| 4 | $[\frac{3}{8}, \frac{3}{8}, \frac{1}{8}]$ | [5, 15, 45, 186] |
| 5 | $[\frac{3}{8}, \frac{1}{8}, \frac{3}{8}]$ | [6, 11, 48, 137] |
| 6 | $[\frac{3}{8}, \frac{5}{8}, \frac{3}{8}]$ | [7, 12, 92, 190] |
| 7 | $[\frac{3}{8}, \frac{1}{8}, \frac{1}{8}]$ | [9, 10, 37, 86] |
| 8 | $[\frac{5}{8}, \frac{3}{8}, \frac{3}{8}]$ | [13, 14, 130, 177] |
| 9 | $[\frac{1}{8}, \frac{7}{8}, \frac{1}{8}]$ | [17, 24, 83, 174] |
| 10 | $[\frac{1}{8}, \frac{1}{8}, \frac{7}{8}]$ | [18, 21, 87, 125] |
| 11 | $[\frac{1}{8}, \frac{1}{8}, \frac{3}{8}]$ | [19, 23, 28, 184] |
| 12 | $[\frac{1}{8}, \frac{3}{8}, \frac{1}{8}]$ | [20, 22, 31, 132] |
| 13 | $[\frac{1}{8}, \frac{7}{8}, \frac{7}{8}]$ | [25, 50, 51, 80] |
| 14 | $[\frac{3}{8}, \frac{5}{8}, \frac{1}{8}]$ | [26, 75, 145, 152] |
| 15 | $[\frac{3}{8}, \frac{1}{8}, \frac{5}{8}]$ | [27, 74, 97, 104] |
| 16 | $[\frac{5}{8}, \frac{1}{8}, \frac{3}{8}]$ | [29, 114, 117, 183] |
| 17 | $[\frac{5}{8}, \frac{3}{8}, \frac{1}{8}]$ | [30, 131, 161, 168] |
| 18 | $[\frac{1}{8}, \frac{7}{8}, \frac{3}{8}]$ | [33, 82, 157, 158] |
| 19 | $[\frac{1}{8}, \frac{3}{8}, \frac{7}{8}]$ | [34, 81, 109, 110] |
| 20 | $[\frac{1}{8}, \frac{3}{8}, \frac{5}{8}]$ | [35, 65, 72, 126] |
| 21 | $[\frac{5}{8}, \frac{3}{8}, \frac{5}{8}]$ | [36, 116, 118, 127] |
| 22 | $[\frac{3}{8}, \frac{5}{8}, \frac{5}{8}]$ | [38, 57, 58, 85] |
| 23 | $[\frac{1}{8}, \frac{5}{8}, \frac{3}{8}]$ | [39, 66, 69, 173] |
| 24 | $[\frac{5}{8}, \frac{5}{8}, \frac{3}{8}]$ | [40, 163, 167, 172] |
| 25 | $[\frac{7}{8}, \frac{1}{8}, \frac{7}{8}]$ | [41, 102, 107, 144] |
| 26 | $[\frac{7}{8}, \frac{7}{8}, \frac{1}{8}]$ | [42, 149, 159, 189] |
| 27 | $[\frac{3}{8}, \frac{7}{8}, \frac{1}{8}]$ | [43, 52, 64, 191] |
| 28 | $[\frac{3}{8}, \frac{1}{8}, \frac{7}{8}]$ | [44, 55, 60, 142] |
| 29 | $[\frac{7}{8}, \frac{1}{8}, \frac{3}{8}]$ | [46, 140, 151, 156] |
| 30 | $[\frac{7}{8}, \frac{3}{8}, \frac{1}{8}]$ | [47, 100, 112, 187] |
| 31 | $[\frac{7}{8}, \frac{5}{8}, \frac{5}{8}]$ | [49, 56, 122, 171] |
| 32 | $[\frac{3}{8}, \frac{7}{8}, \frac{5}{8}]$ | [53, 63, 93, 138] |
| 33 | $[\frac{3}{8}, \frac{5}{8}, \frac{7}{8}]$ | [54, 59, 96, 185] |
| 34 | $[\frac{5}{8}, \frac{7}{8}, \frac{7}{8}]$ | [61, 62, 129, 178] |
| 35 | $[\frac{1}{8}, \frac{5}{8}, \frac{7}{8}]$ | [67, 71, 76, 136] |
| 36 | $[\frac{1}{8}, \frac{7}{8}, \frac{5}{8}]$ | [68, 70, 79, 180] |
| 37 | $[\frac{5}{8}, \frac{5}{8}, \frac{7}{8}]$ | [77, 135, 162, 165] |

continued ...

Table 4

| No. | position | mapping |
|-----|-------------------------------------------|----------------------|
| 38 | $[\frac{5}{8}, \frac{7}{8}, \frac{5}{8}]$ | [78, 113, 120, 179] |
| 39 | $[\frac{5}{8}, \frac{7}{8}, \frac{1}{8}]$ | [84, 164, 166, 175] |
| 40 | $[\frac{5}{8}, \frac{1}{8}, \frac{7}{8}]$ | [88, 115, 119, 124] |
| 41 | $[\frac{7}{8}, \frac{5}{8}, \frac{3}{8}]$ | [89, 150, 155, 192] |
| 42 | $[\frac{7}{8}, \frac{3}{8}, \frac{5}{8}]$ | [90, 101, 111, 141] |
| 43 | $[\frac{7}{8}, \frac{5}{8}, \frac{7}{8}]$ | [94, 103, 108, 188] |
| 44 | $[\frac{7}{8}, \frac{7}{8}, \frac{5}{8}]$ | [95, 139, 148, 160] |
| 45 | $[\frac{5}{8}, \frac{3}{8}, \frac{7}{8}]$ | [98, 99, 128, 169] |
| 46 | $[\frac{7}{8}, \frac{1}{8}, \frac{5}{8}]$ | [105, 106, 133, 182] |
| 47 | $[\frac{5}{8}, \frac{7}{8}, \frac{3}{8}]$ | [121, 146, 147, 176] |
| 48 | $[\frac{7}{8}, \frac{5}{8}, \frac{1}{8}]$ | [134, 153, 154, 181] |

Table 5: Wyckoff site: **64e**, site symmetry: $.3$.

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

continued ...

Table 5

| No. | position | mapping |
|-----|-------------------------------------------------------|---------------|
| 30 | $[x + \frac{1}{4}, \frac{1}{2} - x, x + \frac{3}{4}]$ | [81,91,96] |
| 31 | $[x + \frac{1}{4}, x + \frac{3}{4}, \frac{1}{2} - x]$ | [82,92,93] |
| 32 | $[x + \frac{1}{2}, x, x]$ | [84,86,88] |
| 33 | $[x + \frac{1}{2}, x, x + \frac{1}{2}]$ | [97,113,114] |
| 34 | $[x + \frac{3}{4}, \frac{1}{2} - x, x + \frac{3}{4}]$ | [98,103,111] |
| 35 | $[x + \frac{3}{4}, x + \frac{1}{4}, -x]$ | [99,100,107] |
| 36 | $[-x, x + \frac{1}{4}, x + \frac{3}{4}]$ | [101,102,109] |
| 37 | $[x + \frac{1}{2}, \frac{1}{4} - x, \frac{3}{4} - x]$ | [104,118,119] |
| 38 | $[\frac{3}{4} - x, x, \frac{3}{4} - x]$ | [105,115,120] |
| 39 | $[\frac{3}{4} - x, \frac{1}{4} - x, x + \frac{1}{2}]$ | [106,116,117] |
| 40 | $[-x, \frac{1}{2} - x, -x]$ | [108,110,112] |
| 41 | $[\frac{1}{2} - x, -x, \frac{1}{2} - x]$ | [121,137,138] |
| 42 | $[\frac{3}{4} - x, x + \frac{1}{2}, \frac{3}{4} - x]$ | [122,127,135] |
| 43 | $[\frac{3}{4} - x, \frac{1}{4} - x, x]$ | [123,124,131] |
| 44 | $[x, \frac{1}{4} - x, \frac{3}{4} - x]$ | [125,126,133] |
| 45 | $[\frac{1}{2} - x, x + \frac{1}{4}, x + \frac{3}{4}]$ | [128,142,143] |
| 46 | $[x + \frac{3}{4}, -x, x + \frac{3}{4}]$ | [129,139,144] |
| 47 | $[x + \frac{3}{4}, x + \frac{1}{4}, \frac{1}{2} - x]$ | [130,140,141] |
| 48 | $[x, x + \frac{1}{2}, x]$ | [132,134,136] |
| 49 | $[x + \frac{1}{2}, x + \frac{1}{2}, x]$ | [145,161,162] |
| 50 | $[x + \frac{3}{4}, -x, x + \frac{1}{4}]$ | [146,151,159] |
| 51 | $[x + \frac{3}{4}, x + \frac{3}{4}, \frac{1}{2} - x]$ | [147,148,155] |
| 52 | $[-x, x + \frac{3}{4}, x + \frac{1}{4}]$ | [149,150,157] |
| 53 | $[x + \frac{1}{2}, \frac{3}{4} - x, \frac{1}{4} - x]$ | [152,166,167] |
| 54 | $[\frac{3}{4} - x, x + \frac{1}{2}, \frac{1}{4} - x]$ | [153,163,168] |
| 55 | $[\frac{3}{4} - x, \frac{3}{4} - x, x]$ | [154,164,165] |
| 56 | $[-x, -x, \frac{1}{2} - x]$ | [156,158,160] |
| 57 | $[\frac{1}{2} - x, \frac{1}{2} - x, -x]$ | [169,185,186] |
| 58 | $[\frac{3}{4} - x, x, \frac{1}{4} - x]$ | [170,175,183] |
| 59 | $[\frac{3}{4} - x, \frac{3}{4} - x, x + \frac{1}{2}]$ | [171,172,179] |
| 60 | $[x, \frac{3}{4} - x, \frac{1}{4} - x]$ | [173,174,181] |
| 61 | $[\frac{1}{2} - x, x + \frac{3}{4}, x + \frac{1}{4}]$ | [176,190,191] |
| 62 | $[x + \frac{3}{4}, \frac{1}{2} - x, x + \frac{1}{4}]$ | [177,187,192] |
| 63 | $[x + \frac{3}{4}, x + \frac{3}{4}, -x]$ | [178,188,189] |
| 64 | $[x, x, x + \frac{1}{2}]$ | [180,182,184] |

Table 6: Wyckoff site: 96f, site symmetry: 2..

| No. | position | mapping |
|-----|-----------------------------------------------|---------|
| 1 | $[x, \frac{1}{8}, \frac{1}{8}]$ | [1,8] |
| 2 | $[x + \frac{1}{4}, \frac{3}{8}, \frac{3}{8}]$ | [2,3] |
| 3 | $[\frac{3}{8}, \frac{3}{8}, \frac{1}{2} - x]$ | [4,16] |
| 4 | $[\frac{3}{8}, \frac{3}{8}, x + \frac{1}{4}]$ | [5,15] |
| 5 | $[\frac{3}{8}, x + \frac{1}{4}, \frac{3}{8}]$ | [6,11] |

continued ...

Table 6

| No. | position | mapping |
|-----|-----------------------------------------------|-----------|
| 6 | $[\frac{3}{8}, \frac{1}{2} - x, \frac{3}{8}]$ | [7, 12] |
| 7 | $[\frac{1}{4} - x, \frac{1}{8}, \frac{1}{8}]$ | [9, 10] |
| 8 | $[\frac{1}{2} - x, \frac{3}{8}, \frac{3}{8}]$ | [13, 14] |
| 9 | $[\frac{1}{8}, x, \frac{1}{8}]$ | [17, 24] |
| 10 | $[\frac{1}{8}, \frac{1}{8}, x]$ | [18, 21] |
| 11 | $[\frac{1}{8}, \frac{1}{8}, \frac{1}{4} - x]$ | [19, 23] |
| 12 | $[\frac{1}{8}, \frac{1}{4} - x, \frac{1}{8}]$ | [20, 22] |
| 13 | $[-x, \frac{7}{8}, \frac{7}{8}]$ | [25, 80] |
| 14 | $[\frac{1}{4} - x, \frac{5}{8}, \frac{1}{8}]$ | [26, 75] |
| 15 | $[\frac{1}{4} - x, \frac{1}{8}, \frac{5}{8}]$ | [27, 74] |
| 16 | $[\frac{1}{8}, \frac{1}{8}, x + \frac{1}{2}]$ | [28, 184] |
| 17 | $[\frac{5}{8}, \frac{1}{8}, \frac{1}{4} - x]$ | [29, 183] |
| 18 | $[\frac{5}{8}, \frac{1}{4} - x, \frac{1}{8}]$ | [30, 131] |
| 19 | $[\frac{1}{8}, x + \frac{1}{2}, \frac{1}{8}]$ | [31, 132] |
| 20 | $[-x, \frac{3}{8}, \frac{3}{8}]$ | [32, 73] |
| 21 | $[x + \frac{1}{4}, \frac{7}{8}, \frac{3}{8}]$ | [33, 82] |
| 22 | $[x + \frac{1}{4}, \frac{3}{8}, \frac{7}{8}]$ | [34, 81] |
| 23 | $[\frac{1}{8}, \frac{1}{4} - x, \frac{5}{8}]$ | [35, 126] |
| 24 | $[\frac{5}{8}, x + \frac{1}{2}, \frac{5}{8}]$ | [36, 127] |
| 25 | $[x + \frac{1}{2}, \frac{1}{8}, \frac{1}{8}]$ | [37, 86] |
| 26 | $[x + \frac{1}{2}, \frac{5}{8}, \frac{5}{8}]$ | [38, 85] |
| 27 | $[\frac{1}{8}, \frac{5}{8}, \frac{1}{4} - x]$ | [39, 173] |
| 28 | $[\frac{5}{8}, \frac{5}{8}, x + \frac{1}{2}]$ | [40, 172] |
| 29 | $[\frac{7}{8}, -x, \frac{7}{8}]$ | [41, 144] |
| 30 | $[\frac{7}{8}, \frac{7}{8}, -x]$ | [42, 189] |
| 31 | $[\frac{3}{8}, \frac{7}{8}, x + \frac{1}{4}]$ | [43, 191] |
| 32 | $[\frac{3}{8}, x + \frac{1}{4}, \frac{7}{8}]$ | [44, 142] |
| 33 | $[\frac{3}{8}, \frac{3}{8}, -x]$ | [45, 186] |
| 34 | $[\frac{7}{8}, x + \frac{1}{4}, \frac{3}{8}]$ | [46, 140] |
| 35 | $[\frac{7}{8}, \frac{3}{8}, x + \frac{1}{4}]$ | [47, 187] |
| 36 | $[\frac{3}{8}, -x, \frac{3}{8}]$ | [48, 137] |
| 37 | $[x, \frac{5}{8}, \frac{5}{8}]$ | [49, 56] |
| 38 | $[x + \frac{1}{4}, \frac{7}{8}, \frac{7}{8}]$ | [50, 51] |
| 39 | $[\frac{3}{8}, \frac{7}{8}, -x]$ | [52, 64] |
| 40 | $[\frac{3}{8}, \frac{7}{8}, x + \frac{3}{4}]$ | [53, 63] |
| 41 | $[\frac{3}{8}, x + \frac{3}{4}, \frac{7}{8}]$ | [54, 59] |
| 42 | $[\frac{3}{8}, -x, \frac{7}{8}]$ | [55, 60] |
| 43 | $[\frac{1}{4} - x, \frac{5}{8}, \frac{5}{8}]$ | [57, 58] |
| 44 | $[\frac{1}{2} - x, \frac{7}{8}, \frac{7}{8}]$ | [61, 62] |
| 45 | $[\frac{1}{8}, x + \frac{1}{2}, \frac{5}{8}]$ | [65, 72] |
| 46 | $[\frac{1}{8}, \frac{5}{8}, x + \frac{1}{2}]$ | [66, 69] |
| 47 | $[\frac{1}{8}, \frac{5}{8}, \frac{3}{4} - x]$ | [67, 71] |
| 48 | $[\frac{1}{8}, \frac{3}{4} - x, \frac{5}{8}]$ | [68, 70] |
| 49 | $[\frac{1}{8}, \frac{5}{8}, x]$ | [76, 136] |
| 50 | $[\frac{5}{8}, \frac{5}{8}, \frac{3}{4} - x]$ | [77, 135] |
| 51 | $[\frac{5}{8}, \frac{3}{4} - x, \frac{5}{8}]$ | [78, 179] |
| 52 | $[\frac{1}{8}, x, \frac{5}{8}]$ | [79, 180] |

continued ...

Table 6

| No. | position | mapping |
|-----|-----------------------------------------------|------------|
| 53 | $[\frac{1}{8}, \frac{3}{4} - x, \frac{1}{8}]$ | [83, 174] |
| 54 | $[\frac{5}{8}, x, \frac{1}{8}]$ | [84, 175] |
| 55 | $[\frac{1}{8}, \frac{1}{8}, \frac{3}{4} - x]$ | [87, 125] |
| 56 | $[\frac{5}{8}, \frac{1}{8}, x]$ | [88, 124] |
| 57 | $[\frac{7}{8}, \frac{1}{2} - x, \frac{3}{8}]$ | [89, 192] |
| 58 | $[\frac{7}{8}, \frac{3}{8}, \frac{1}{2} - x]$ | [90, 141] |
| 59 | $[\frac{3}{8}, \frac{3}{8}, x + \frac{3}{4}]$ | [91, 143] |
| 60 | $[\frac{3}{8}, x + \frac{3}{4}, \frac{3}{8}]$ | [92, 190] |
| 61 | $[\frac{3}{8}, \frac{7}{8}, \frac{1}{2} - x]$ | [93, 138] |
| 62 | $[\frac{7}{8}, x + \frac{3}{4}, \frac{7}{8}]$ | [94, 188] |
| 63 | $[\frac{7}{8}, \frac{7}{8}, x + \frac{3}{4}]$ | [95, 139] |
| 64 | $[\frac{3}{8}, \frac{1}{2} - x, \frac{7}{8}]$ | [96, 185] |
| 65 | $[x + \frac{1}{2}, \frac{1}{8}, \frac{5}{8}]$ | [97, 104] |
| 66 | $[x + \frac{3}{4}, \frac{3}{8}, \frac{7}{8}]$ | [98, 99] |
| 67 | $[\frac{7}{8}, \frac{3}{8}, -x]$ | [100, 112] |
| 68 | $[\frac{7}{8}, \frac{3}{8}, x + \frac{3}{4}]$ | [101, 111] |
| 69 | $[\frac{7}{8}, x + \frac{1}{4}, \frac{7}{8}]$ | [102, 107] |
| 70 | $[\frac{7}{8}, \frac{1}{2} - x, \frac{7}{8}]$ | [103, 108] |
| 71 | $[\frac{3}{4} - x, \frac{1}{8}, \frac{5}{8}]$ | [105, 106] |
| 72 | $[-x, \frac{3}{8}, \frac{7}{8}]$ | [109, 110] |
| 73 | $[\frac{5}{8}, x, \frac{5}{8}]$ | [113, 120] |
| 74 | $[\frac{5}{8}, \frac{1}{8}, x + \frac{1}{2}]$ | [114, 117] |
| 75 | $[\frac{5}{8}, \frac{1}{8}, \frac{3}{4} - x]$ | [115, 119] |
| 76 | $[\frac{5}{8}, \frac{1}{4} - x, \frac{5}{8}]$ | [116, 118] |
| 77 | $[\frac{1}{2} - x, \frac{7}{8}, \frac{3}{8}]$ | [121, 176] |
| 78 | $[\frac{3}{4} - x, \frac{5}{8}, \frac{5}{8}]$ | [122, 171] |
| 79 | $[\frac{3}{4} - x, \frac{1}{8}, \frac{1}{8}]$ | [123, 170] |
| 80 | $[\frac{1}{2} - x, \frac{3}{8}, \frac{7}{8}]$ | [128, 169] |
| 81 | $[x + \frac{3}{4}, \frac{7}{8}, \frac{7}{8}]$ | [129, 178] |
| 82 | $[x + \frac{3}{4}, \frac{3}{8}, \frac{3}{8}]$ | [130, 177] |
| 83 | $[x, \frac{1}{8}, \frac{5}{8}]$ | [133, 182] |
| 84 | $[x, \frac{5}{8}, \frac{1}{8}]$ | [134, 181] |
| 85 | $[x + \frac{1}{2}, \frac{5}{8}, \frac{1}{8}]$ | [145, 152] |
| 86 | $[x + \frac{3}{4}, \frac{7}{8}, \frac{3}{8}]$ | [146, 147] |
| 87 | $[\frac{7}{8}, \frac{7}{8}, \frac{1}{2} - x]$ | [148, 160] |
| 88 | $[\frac{7}{8}, \frac{7}{8}, x + \frac{1}{4}]$ | [149, 159] |
| 89 | $[\frac{7}{8}, x + \frac{3}{4}, \frac{3}{8}]$ | [150, 155] |
| 90 | $[\frac{7}{8}, -x, \frac{3}{8}]$ | [151, 156] |
| 91 | $[\frac{3}{4} - x, \frac{5}{8}, \frac{1}{8}]$ | [153, 154] |
| 92 | $[-x, \frac{7}{8}, \frac{3}{8}]$ | [157, 158] |
| 93 | $[\frac{5}{8}, x + \frac{1}{2}, \frac{1}{8}]$ | [161, 168] |
| 94 | $[\frac{5}{8}, \frac{5}{8}, x]$ | [162, 165] |
| 95 | $[\frac{5}{8}, \frac{5}{8}, \frac{1}{4} - x]$ | [163, 167] |
| 96 | $[\frac{5}{8}, \frac{3}{4} - x, \frac{1}{8}]$ | [164, 166] |

Table 7: Wyckoff site: 96g, site symmetry: $\dots 2$

| No. | position | mapping |
|-----|---------------------------------------------------|----------|
| 1 | $[\frac{1}{4}, y, -y]$ | [1,62] |
| 2 | $[\frac{1}{2}, y + \frac{1}{2}, y + \frac{1}{4}]$ | [2,153] |
| 3 | $[\frac{1}{2}, \frac{1}{4} - y, \frac{1}{2} - y]$ | [3,106] |
| 4 | $[\frac{1}{4} - y, y + \frac{1}{4}, \frac{1}{4}]$ | [4,21] |
| 5 | $[y + \frac{1}{2}, y + \frac{1}{4}, \frac{1}{2}]$ | [5,119] |
| 6 | $[\frac{1}{2} - y, \frac{1}{2}, \frac{1}{4} - y]$ | [6,166] |
| 7 | $[y + \frac{1}{4}, \frac{1}{4}, \frac{1}{4} - y]$ | [7,24] |
| 8 | $[\frac{1}{4}, \frac{1}{4} - y, y + \frac{1}{4}]$ | [8,13] |
| 9 | $[0, y, y + \frac{1}{4}]$ | [9,146] |
| 10 | $[0, \frac{1}{4} - y, -y]$ | [10,99] |
| 11 | $[y + \frac{1}{4}, \frac{1}{2}, y + \frac{1}{2}]$ | [11,68] |
| 12 | $[\frac{1}{2} - y, \frac{1}{4}, y + \frac{1}{2}]$ | [12,113] |
| 13 | $[\frac{1}{4}, y + \frac{1}{2}, \frac{1}{2} - y]$ | [14,49] |
| 14 | $[\frac{1}{4} - y, \frac{1}{2} - y, \frac{1}{2}]$ | [15,67] |
| 15 | $[y + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{4}]$ | [16,162] |
| 16 | $[-y, \frac{1}{4}, y]$ | [17,108] |
| 17 | $[y, -y, \frac{1}{4}]$ | [18,160] |
| 18 | $[\frac{1}{4} - y, -y, 0]$ | [19,63] |
| 19 | $[y + \frac{1}{4}, 0, y]$ | [20,59] |
| 20 | $[-y, 0, \frac{1}{4} - y]$ | [22,150] |
| 21 | $[y, y + \frac{1}{4}, 0]$ | [23,101] |
| 22 | $[\frac{3}{4}, -y, y]$ | [25,86] |
| 23 | $[0, \frac{1}{2} - y, \frac{1}{4} - y]$ | [26,177] |
| 24 | $[0, y + \frac{1}{4}, y + \frac{1}{2}]$ | [27,130] |
| 25 | $[y + \frac{1}{4}, \frac{1}{4} - y, \frac{3}{4}]$ | [28,45] |
| 26 | $[\frac{1}{2} - y, \frac{1}{4} - y, 0]$ | [29,143] |
| 27 | $[y + \frac{1}{2}, 0, y + \frac{1}{4}]$ | [30,190] |
| 28 | $[\frac{1}{4} - y, \frac{3}{4}, y + \frac{1}{4}]$ | [31,48] |
| 29 | $[\frac{3}{4}, y + \frac{1}{4}, \frac{1}{4} - y]$ | [32,37] |
| 30 | $[\frac{1}{2}, -y, \frac{1}{4} - y]$ | [33,170] |
| 31 | $[\frac{1}{2}, y + \frac{1}{4}, y]$ | [34,123] |
| 32 | $[\frac{1}{4} - y, 0, \frac{1}{2} - y]$ | [35,92] |
| 33 | $[y + \frac{1}{2}, \frac{3}{4}, \frac{1}{2} - y]$ | [36,137] |
| 34 | $[\frac{3}{4}, \frac{1}{2} - y, y + \frac{1}{2}]$ | [38,73] |
| 35 | $[y + \frac{1}{4}, y + \frac{1}{2}, 0]$ | [39,91] |
| 36 | $[\frac{1}{2} - y, y + \frac{1}{2}, \frac{3}{4}]$ | [40,186] |
| 37 | $[y, \frac{3}{4}, -y]$ | [41,132] |
| 38 | $[-y, y, \frac{3}{4}]$ | [42,184] |
| 39 | $[y + \frac{1}{4}, y, \frac{1}{2}]$ | [43,87] |
| 40 | $[\frac{1}{4} - y, \frac{1}{2}, -y]$ | [44,83] |
| 41 | $[y, \frac{1}{2}, y + \frac{1}{4}]$ | [46,174] |
| 42 | $[-y, \frac{1}{4} - y, \frac{1}{2}]$ | [47,125] |
| 43 | $[\frac{1}{2}, y, y + \frac{3}{4}]$ | [50,105] |
| 44 | $[\frac{1}{2}, \frac{3}{4} - y, -y]$ | [51,154] |
| 45 | $[\frac{1}{4} - y, y + \frac{3}{4}, \frac{3}{4}]$ | [52,69] |
| 46 | $[y + \frac{1}{2}, y + \frac{3}{4}, 0]$ | [53,167] |

continued ...

Table 7

| No. | position | mapping |
|-----|---------------------------------------------------|------------|
| 47 | $[\frac{1}{2} - y, 0, \frac{3}{4} - y]$ | [54, 118] |
| 48 | $[y + \frac{1}{4}, \frac{3}{4}, \frac{3}{4} - y]$ | [55, 72] |
| 49 | $[\frac{1}{4}, \frac{3}{4} - y, y + \frac{3}{4}]$ | [56, 61] |
| 50 | $[0, y + \frac{1}{2}, y + \frac{3}{4}]$ | [57, 98] |
| 51 | $[0, \frac{3}{4} - y, \frac{1}{2} - y]$ | [58, 147] |
| 52 | $[\frac{1}{2} - y, \frac{3}{4}, y]$ | [60, 161] |
| 53 | $[y + \frac{1}{2}, -y, \frac{3}{4}]$ | [64, 114] |
| 54 | $[-y, \frac{3}{4}, y + \frac{1}{2}]$ | [65, 156] |
| 55 | $[y, \frac{1}{2} - y, \frac{3}{4}]$ | [66, 112] |
| 56 | $[-y, \frac{1}{2}, \frac{3}{4} - y]$ | [70, 102] |
| 57 | $[y, y + \frac{3}{4}, \frac{1}{2}]$ | [71, 149] |
| 58 | $[0, -y, \frac{3}{4} - y]$ | [74, 129] |
| 59 | $[0, y + \frac{3}{4}, y]$ | [75, 178] |
| 60 | $[y + \frac{1}{4}, \frac{3}{4} - y, \frac{1}{4}]$ | [76, 93] |
| 61 | $[\frac{1}{2} - y, \frac{3}{4} - y, \frac{1}{2}]$ | [77, 191] |
| 62 | $[y + \frac{1}{2}, \frac{1}{2}, y + \frac{3}{4}]$ | [78, 142] |
| 63 | $[\frac{1}{4} - y, \frac{1}{4}, y + \frac{3}{4}]$ | [79, 96] |
| 64 | $[\frac{3}{4}, y + \frac{3}{4}, \frac{3}{4} - y]$ | [80, 85] |
| 65 | $[\frac{1}{2}, \frac{1}{2} - y, \frac{3}{4} - y]$ | [81, 122] |
| 66 | $[\frac{1}{2}, y + \frac{3}{4}, y + \frac{1}{2}]$ | [82, 171] |
| 67 | $[y + \frac{1}{2}, \frac{1}{4}, -y]$ | [84, 185] |
| 68 | $[\frac{1}{2} - y, y, \frac{1}{4}]$ | [88, 138] |
| 69 | $[y, \frac{1}{4}, \frac{1}{2} - y]$ | [89, 180] |
| 70 | $[-y, y + \frac{1}{2}, \frac{1}{4}]$ | [90, 136] |
| 71 | $[y, 0, y + \frac{3}{4}]$ | [94, 126] |
| 72 | $[-y, \frac{3}{4} - y, 0]$ | [95, 173] |
| 73 | $[\frac{3}{4}, y, \frac{1}{2} - y]$ | [97, 158] |
| 74 | $[\frac{3}{4} - y, y + \frac{1}{4}, \frac{3}{4}]$ | [100, 117] |
| 75 | $[y + \frac{3}{4}, \frac{1}{4}, \frac{3}{4} - y]$ | [103, 120] |
| 76 | $[\frac{3}{4}, \frac{1}{4} - y, y + \frac{3}{4}]$ | [104, 109] |
| 77 | $[y + \frac{3}{4}, \frac{1}{2}, y]$ | [107, 164] |
| 78 | $[\frac{3}{4}, y + \frac{1}{2}, -y]$ | [110, 145] |
| 79 | $[\frac{3}{4} - y, \frac{1}{2} - y, 0]$ | [111, 163] |
| 80 | $[\frac{3}{4} - y, -y, \frac{1}{2}]$ | [115, 159] |
| 81 | $[y + \frac{3}{4}, 0, y + \frac{1}{2}]$ | [116, 155] |
| 82 | $[\frac{1}{4}, -y, y + \frac{1}{2}]$ | [121, 182] |
| 83 | $[y + \frac{3}{4}, \frac{1}{4} - y, \frac{1}{4}]$ | [124, 141] |
| 84 | $[\frac{3}{4} - y, \frac{3}{4}, y + \frac{3}{4}]$ | [127, 144] |
| 85 | $[\frac{1}{4}, y + \frac{1}{4}, \frac{3}{4} - y]$ | [128, 133] |
| 86 | $[\frac{3}{4} - y, 0, -y]$ | [131, 188] |
| 87 | $[\frac{1}{4}, \frac{1}{2} - y, y]$ | [134, 169] |
| 88 | $[y + \frac{3}{4}, y + \frac{1}{2}, \frac{1}{2}]$ | [135, 187] |
| 89 | $[y + \frac{3}{4}, y, 0]$ | [139, 183] |
| 90 | $[\frac{3}{4} - y, \frac{1}{2}, \frac{1}{2} - y]$ | [140, 179] |
| 91 | $[\frac{3}{4} - y, y + \frac{3}{4}, \frac{1}{4}]$ | [148, 165] |
| 92 | $[y + \frac{3}{4}, \frac{3}{4}, \frac{1}{4} - y]$ | [151, 168] |
| 93 | $[\frac{3}{4}, \frac{3}{4} - y, y + \frac{1}{4}]$ | [152, 157] |

continued ...

Table 7

| No. | position | mapping |
|-----|---------------------------------------------------|-----------|
| 94 | $[y + \frac{3}{4}, \frac{3}{4} - y, \frac{3}{4}]$ | [172,189] |
| 95 | $[\frac{3}{4} - y, \frac{1}{4}, y + \frac{1}{4}]$ | [175,192] |
| 96 | $[\frac{1}{4}, y + \frac{3}{4}, \frac{1}{4} - y]$ | [176,181] |

Table 8: Wyckoff site: 192h, site symmetry: 1

| No. | position | mapping |
|-----|-------------------------------------------------------|---------|
| 1 | $[x, y, z]$ | [1] |
| 2 | $[x + \frac{1}{4}, \frac{1}{2} - z, y + \frac{1}{4}]$ | [2] |
| 3 | $[x + \frac{1}{4}, z + \frac{1}{4}, \frac{1}{2} - y]$ | [3] |
| 4 | $[z + \frac{1}{4}, y + \frac{1}{4}, \frac{1}{2} - x]$ | [4] |
| 5 | $[\frac{1}{2} - z, y + \frac{1}{4}, x + \frac{1}{4}]$ | [5] |
| 6 | $[\frac{1}{2} - y, x + \frac{1}{4}, z + \frac{1}{4}]$ | [6] |
| 7 | $[y + \frac{1}{4}, \frac{1}{2} - x, z + \frac{1}{4}]$ | [7] |
| 8 | $[x, \frac{1}{4} - y, \frac{1}{4} - z]$ | [8] |
| 9 | $[\frac{1}{4} - x, y, \frac{1}{4} - z]$ | [9] |
| 10 | $[\frac{1}{4} - x, \frac{1}{4} - y, z]$ | [10] |
| 11 | $[y + \frac{1}{4}, x + \frac{1}{4}, \frac{1}{2} - z]$ | [11] |
| 12 | $[\frac{1}{2} - y, \frac{1}{2} - x, \frac{1}{2} - z]$ | [12] |
| 13 | $[\frac{1}{2} - x, z + \frac{1}{4}, y + \frac{1}{4}]$ | [13] |
| 14 | $[\frac{1}{2} - x, \frac{1}{2} - z, \frac{1}{2} - y]$ | [14] |
| 15 | $[z + \frac{1}{4}, \frac{1}{2} - y, x + \frac{1}{4}]$ | [15] |
| 16 | $[\frac{1}{2} - z, \frac{1}{2} - y, \frac{1}{2} - x]$ | [16] |
| 17 | $[z, x, y]$ | [17] |
| 18 | $[y, z, x]$ | [18] |
| 19 | $[\frac{1}{4} - y, z, \frac{1}{4} - x]$ | [19] |
| 20 | $[\frac{1}{4} - z, \frac{1}{4} - x, y]$ | [20] |
| 21 | $[\frac{1}{4} - y, \frac{1}{4} - z, x]$ | [21] |
| 22 | $[z, \frac{1}{4} - x, \frac{1}{4} - y]$ | [22] |
| 23 | $[y, \frac{1}{4} - z, \frac{1}{4} - x]$ | [23] |
| 24 | $[\frac{1}{4} - z, x, \frac{1}{4} - y]$ | [24] |
| 25 | $[-x, -y, -z]$ | [25] |
| 26 | $[\frac{1}{4} - x, z + \frac{1}{2}, \frac{1}{4} - y]$ | [26] |
| 27 | $[\frac{1}{4} - x, \frac{1}{4} - z, y + \frac{1}{2}]$ | [27] |
| 28 | $[\frac{1}{4} - z, \frac{1}{4} - y, x + \frac{1}{2}]$ | [28] |
| 29 | $[z + \frac{1}{2}, \frac{1}{4} - y, \frac{1}{4} - x]$ | [29] |
| 30 | $[y + \frac{1}{2}, \frac{1}{4} - x, \frac{1}{4} - z]$ | [30] |
| 31 | $[\frac{1}{4} - y, x + \frac{1}{2}, \frac{1}{4} - z]$ | [31] |
| 32 | $[-x, y + \frac{1}{4}, z + \frac{1}{4}]$ | [32] |
| 33 | $[x + \frac{1}{4}, -y, z + \frac{1}{4}]$ | [33] |
| 34 | $[x + \frac{1}{4}, y + \frac{1}{4}, -z]$ | [34] |
| 35 | $[\frac{1}{4} - y, \frac{1}{4} - x, z + \frac{1}{2}]$ | [35] |
| 36 | $[y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}]$ | [36] |
| 37 | $[x + \frac{1}{2}, \frac{1}{4} - z, \frac{1}{4} - y]$ | [37] |

continued ...

Table 8

| No. | position | mapping |
|-----|-------------------------------------------------------|---------|
| 38 | $[x + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}]$ | [38] |
| 39 | $[\frac{1}{4} - z, y + \frac{1}{2}, \frac{1}{4} - x]$ | [39] |
| 40 | $[z + \frac{1}{2}, y + \frac{1}{2}, x + \frac{1}{2}]$ | [40] |
| 41 | $[-z, -x, -y]$ | [41] |
| 42 | $[-y, -z, -x]$ | [42] |
| 43 | $[y + \frac{1}{4}, -z, x + \frac{1}{4}]$ | [43] |
| 44 | $[z + \frac{1}{4}, x + \frac{1}{4}, -y]$ | [44] |
| 45 | $[y + \frac{1}{4}, z + \frac{1}{4}, -x]$ | [45] |
| 46 | $[-z, x + \frac{1}{4}, y + \frac{1}{4}]$ | [46] |
| 47 | $[-y, z + \frac{1}{4}, x + \frac{1}{4}]$ | [47] |
| 48 | $[z + \frac{1}{4}, -x, y + \frac{1}{4}]$ | [48] |
| 49 | $[x, y + \frac{1}{2}, z + \frac{1}{2}]$ | [49] |
| 50 | $[x + \frac{1}{4}, -z, y + \frac{3}{4}]$ | [50] |
| 51 | $[x + \frac{1}{4}, z + \frac{3}{4}, -y]$ | [51] |
| 52 | $[z + \frac{1}{4}, y + \frac{3}{4}, -x]$ | [52] |
| 53 | $[\frac{1}{2} - z, y + \frac{3}{4}, x + \frac{3}{4}]$ | [53] |
| 54 | $[\frac{1}{2} - y, x + \frac{3}{4}, z + \frac{3}{4}]$ | [54] |
| 55 | $[y + \frac{1}{4}, -x, z + \frac{3}{4}]$ | [55] |
| 56 | $[x, \frac{3}{4} - y, \frac{3}{4} - z]$ | [56] |
| 57 | $[\frac{1}{4} - x, y + \frac{1}{2}, \frac{3}{4} - z]$ | [57] |
| 58 | $[\frac{1}{4} - x, \frac{3}{4} - y, z + \frac{1}{2}]$ | [58] |
| 59 | $[y + \frac{1}{4}, x + \frac{3}{4}, -z]$ | [59] |
| 60 | $[\frac{1}{2} - y, -x, -z]$ | [60] |
| 61 | $[\frac{1}{2} - x, z + \frac{3}{4}, y + \frac{3}{4}]$ | [61] |
| 62 | $[\frac{1}{2} - x, -z, -y]$ | [62] |
| 63 | $[z + \frac{1}{4}, -y, x + \frac{3}{4}]$ | [63] |
| 64 | $[\frac{1}{2} - z, -y, -x]$ | [64] |
| 65 | $[z, x + \frac{1}{2}, y + \frac{1}{2}]$ | [65] |
| 66 | $[y, z + \frac{1}{2}, x + \frac{1}{2}]$ | [66] |
| 67 | $[\frac{1}{4} - y, z + \frac{1}{2}, \frac{3}{4} - x]$ | [67] |
| 68 | $[\frac{1}{4} - z, \frac{3}{4} - x, y + \frac{1}{2}]$ | [68] |
| 69 | $[\frac{1}{4} - y, \frac{3}{4} - z, x + \frac{1}{2}]$ | [69] |
| 70 | $[z, \frac{3}{4} - x, \frac{3}{4} - y]$ | [70] |
| 71 | $[y, \frac{3}{4} - z, \frac{3}{4} - x]$ | [71] |
| 72 | $[\frac{1}{4} - z, x + \frac{1}{2}, \frac{3}{4} - y]$ | [72] |
| 73 | $[-x, \frac{1}{2} - y, \frac{1}{2} - z]$ | [73] |
| 74 | $[\frac{1}{4} - x, z, \frac{3}{4} - y]$ | [74] |
| 75 | $[\frac{1}{4} - x, \frac{3}{4} - z, y]$ | [75] |
| 76 | $[\frac{1}{4} - z, \frac{3}{4} - y, x]$ | [76] |
| 77 | $[z + \frac{1}{2}, \frac{3}{4} - y, \frac{3}{4} - x]$ | [77] |
| 78 | $[y + \frac{1}{2}, \frac{3}{4} - x, \frac{3}{4} - z]$ | [78] |
| 79 | $[\frac{1}{4} - y, x, \frac{3}{4} - z]$ | [79] |
| 80 | $[-x, y + \frac{3}{4}, z + \frac{3}{4}]$ | [80] |
| 81 | $[x + \frac{1}{4}, \frac{1}{2} - y, z + \frac{3}{4}]$ | [81] |
| 82 | $[x + \frac{1}{4}, y + \frac{3}{4}, \frac{1}{2} - z]$ | [82] |
| 83 | $[\frac{1}{4} - y, \frac{3}{4} - x, z]$ | [83] |
| 84 | $[y + \frac{1}{2}, x, z]$ | [84] |

continued ...

Table 8

| No. | position | mapping |
|-----|-------------------------------------------------------|---------|
| 85 | $[x + \frac{1}{2}, \frac{3}{4} - z, \frac{3}{4} - y]$ | [85] |
| 86 | $[x + \frac{1}{2}, z, y]$ | [86] |
| 87 | $[\frac{1}{4} - z, y, \frac{3}{4} - x]$ | [87] |
| 88 | $[z + \frac{1}{2}, y, x]$ | [88] |
| 89 | $[-z, \frac{1}{2} - x, \frac{1}{2} - y]$ | [89] |
| 90 | $[-y, \frac{1}{2} - z, \frac{1}{2} - x]$ | [90] |
| 91 | $[y + \frac{1}{4}, \frac{1}{2} - z, x + \frac{3}{4}]$ | [91] |
| 92 | $[z + \frac{1}{4}, x + \frac{3}{4}, \frac{1}{2} - y]$ | [92] |
| 93 | $[y + \frac{1}{4}, z + \frac{3}{4}, \frac{1}{2} - x]$ | [93] |
| 94 | $[-z, x + \frac{3}{4}, y + \frac{3}{4}]$ | [94] |
| 95 | $[-y, z + \frac{3}{4}, x + \frac{3}{4}]$ | [95] |
| 96 | $[z + \frac{1}{4}, \frac{1}{2} - x, y + \frac{3}{4}]$ | [96] |
| 97 | $[x + \frac{1}{2}, y, z + \frac{1}{2}]$ | [97] |
| 98 | $[x + \frac{3}{4}, \frac{1}{2} - z, y + \frac{3}{4}]$ | [98] |
| 99 | $[x + \frac{3}{4}, z + \frac{1}{4}, -y]$ | [99] |
| 100 | $[z + \frac{3}{4}, y + \frac{1}{4}, -x]$ | [100] |
| 101 | $[-z, y + \frac{1}{4}, x + \frac{3}{4}]$ | [101] |
| 102 | $[-y, x + \frac{1}{4}, z + \frac{3}{4}]$ | [102] |
| 103 | $[y + \frac{3}{4}, \frac{1}{2} - x, z + \frac{3}{4}]$ | [103] |
| 104 | $[x + \frac{1}{2}, \frac{1}{4} - y, \frac{3}{4} - z]$ | [104] |
| 105 | $[\frac{3}{4} - x, y, \frac{3}{4} - z]$ | [105] |
| 106 | $[\frac{3}{4} - x, \frac{1}{4} - y, z + \frac{1}{2}]$ | [106] |
| 107 | $[y + \frac{3}{4}, x + \frac{1}{4}, -z]$ | [107] |
| 108 | $[-y, \frac{1}{2} - x, -z]$ | [108] |
| 109 | $[-x, z + \frac{1}{4}, y + \frac{3}{4}]$ | [109] |
| 110 | $[-x, \frac{1}{2} - z, -y]$ | [110] |
| 111 | $[z + \frac{3}{4}, \frac{1}{2} - y, x + \frac{3}{4}]$ | [111] |
| 112 | $[-z, \frac{1}{2} - y, -x]$ | [112] |
| 113 | $[z + \frac{1}{2}, x, y + \frac{1}{2}]$ | [113] |
| 114 | $[y + \frac{1}{2}, z, x + \frac{1}{2}]$ | [114] |
| 115 | $[\frac{3}{4} - y, z, \frac{3}{4} - x]$ | [115] |
| 116 | $[\frac{3}{4} - z, \frac{1}{4} - x, y + \frac{1}{2}]$ | [116] |
| 117 | $[\frac{3}{4} - y, \frac{1}{4} - z, x + \frac{1}{2}]$ | [117] |
| 118 | $[z + \frac{1}{2}, \frac{1}{4} - x, \frac{3}{4} - y]$ | [118] |
| 119 | $[y + \frac{1}{2}, \frac{1}{4} - z, \frac{3}{4} - x]$ | [119] |
| 120 | $[\frac{3}{4} - z, x, \frac{3}{4} - y]$ | [120] |
| 121 | $[\frac{1}{2} - x, -y, \frac{1}{2} - z]$ | [121] |
| 122 | $[\frac{3}{4} - x, z + \frac{1}{2}, \frac{3}{4} - y]$ | [122] |
| 123 | $[\frac{3}{4} - x, \frac{1}{4} - z, y]$ | [123] |
| 124 | $[\frac{3}{4} - z, \frac{1}{4} - y, x]$ | [124] |
| 125 | $[z, \frac{1}{4} - y, \frac{3}{4} - x]$ | [125] |
| 126 | $[y, \frac{1}{4} - x, \frac{3}{4} - z]$ | [126] |
| 127 | $[\frac{3}{4} - y, x + \frac{1}{2}, \frac{3}{4} - z]$ | [127] |
| 128 | $[\frac{1}{2} - x, y + \frac{1}{4}, z + \frac{3}{4}]$ | [128] |
| 129 | $[x + \frac{3}{4}, -y, z + \frac{3}{4}]$ | [129] |
| 130 | $[x + \frac{3}{4}, y + \frac{1}{4}, \frac{1}{2} - z]$ | [130] |
| 131 | $[\frac{3}{4} - y, \frac{1}{4} - x, z]$ | [131] |

continued ...

Table 8

| No. | position | mapping |
|-----|-------------------------------------------------------|---------|
| 132 | $[y, x + \frac{1}{2}, z]$ | [132] |
| 133 | $[x, \frac{1}{4} - z, \frac{3}{4} - y]$ | [133] |
| 134 | $[x, z + \frac{1}{2}, y]$ | [134] |
| 135 | $[\frac{3}{4} - z, y + \frac{1}{2}, \frac{3}{4} - x]$ | [135] |
| 136 | $[z, y + \frac{1}{2}, x]$ | [136] |
| 137 | $[\frac{1}{2} - z, -x, \frac{1}{2} - y]$ | [137] |
| 138 | $[\frac{1}{2} - y, -z, \frac{1}{2} - x]$ | [138] |
| 139 | $[y + \frac{3}{4}, -z, x + \frac{3}{4}]$ | [139] |
| 140 | $[z + \frac{3}{4}, x + \frac{1}{4}, \frac{1}{2} - y]$ | [140] |
| 141 | $[y + \frac{3}{4}, z + \frac{1}{4}, \frac{1}{2} - x]$ | [141] |
| 142 | $[\frac{1}{2} - z, x + \frac{1}{4}, y + \frac{3}{4}]$ | [142] |
| 143 | $[\frac{1}{2} - y, z + \frac{1}{4}, x + \frac{3}{4}]$ | [143] |
| 144 | $[z + \frac{3}{4}, -x, y + \frac{3}{4}]$ | [144] |
| 145 | $[x + \frac{1}{2}, y + \frac{1}{2}, z]$ | [145] |
| 146 | $[x + \frac{3}{4}, -z, y + \frac{1}{4}]$ | [146] |
| 147 | $[x + \frac{3}{4}, z + \frac{3}{4}, \frac{1}{2} - y]$ | [147] |
| 148 | $[z + \frac{3}{4}, y + \frac{3}{4}, \frac{1}{2} - x]$ | [148] |
| 149 | $[-z, y + \frac{3}{4}, x + \frac{1}{4}]$ | [149] |
| 150 | $[-y, x + \frac{3}{4}, z + \frac{1}{4}]$ | [150] |
| 151 | $[y + \frac{3}{4}, -x, z + \frac{1}{4}]$ | [151] |
| 152 | $[x + \frac{1}{2}, \frac{3}{4} - y, \frac{1}{4} - z]$ | [152] |
| 153 | $[\frac{3}{4} - x, y + \frac{1}{2}, \frac{1}{4} - z]$ | [153] |
| 154 | $[\frac{3}{4} - x, \frac{3}{4} - y, z]$ | [154] |
| 155 | $[y + \frac{3}{4}, x + \frac{3}{4}, \frac{1}{2} - z]$ | [155] |
| 156 | $[-y, -x, \frac{1}{2} - z]$ | [156] |
| 157 | $[-x, z + \frac{3}{4}, y + \frac{1}{4}]$ | [157] |
| 158 | $[-x, -z, \frac{1}{2} - y]$ | [158] |
| 159 | $[z + \frac{3}{4}, -y, x + \frac{1}{4}]$ | [159] |
| 160 | $[-z, -y, \frac{1}{2} - x]$ | [160] |
| 161 | $[z + \frac{1}{2}, x + \frac{1}{2}, y]$ | [161] |
| 162 | $[y + \frac{1}{2}, z + \frac{1}{2}, x]$ | [162] |
| 163 | $[\frac{3}{4} - y, z + \frac{1}{2}, \frac{1}{4} - x]$ | [163] |
| 164 | $[\frac{3}{4} - z, \frac{3}{4} - x, y]$ | [164] |
| 165 | $[\frac{3}{4} - y, \frac{3}{4} - z, x]$ | [165] |
| 166 | $[z + \frac{1}{2}, \frac{3}{4} - x, \frac{1}{4} - y]$ | [166] |
| 167 | $[y + \frac{1}{2}, \frac{3}{4} - z, \frac{1}{4} - x]$ | [167] |
| 168 | $[\frac{3}{4} - z, x + \frac{1}{2}, \frac{1}{4} - y]$ | [168] |
| 169 | $[\frac{1}{2} - x, \frac{1}{2} - y, -z]$ | [169] |
| 170 | $[\frac{3}{4} - x, z, \frac{1}{4} - y]$ | [170] |
| 171 | $[\frac{3}{4} - x, \frac{3}{4} - z, y + \frac{1}{2}]$ | [171] |
| 172 | $[\frac{3}{4} - z, \frac{3}{4} - y, x + \frac{1}{2}]$ | [172] |
| 173 | $[z, \frac{3}{4} - y, \frac{1}{4} - x]$ | [173] |
| 174 | $[y, \frac{3}{4} - x, \frac{1}{4} - z]$ | [174] |
| 175 | $[\frac{3}{4} - y, x, \frac{1}{4} - z]$ | [175] |
| 176 | $[\frac{1}{2} - x, y + \frac{3}{4}, z + \frac{1}{4}]$ | [176] |
| 177 | $[x + \frac{3}{4}, \frac{1}{2} - y, z + \frac{1}{4}]$ | [177] |
| 178 | $[x + \frac{3}{4}, y + \frac{3}{4}, -z]$ | [178] |

continued ...

Table 8

| No. | position | mapping |
|-----|-------------------------------------------------------|---------|
| 179 | $[\frac{3}{4} - y, \frac{3}{4} - x, z + \frac{1}{2}]$ | [179] |
| 180 | $[y, x, z + \frac{1}{2}]$ | [180] |
| 181 | $[x, \frac{3}{4} - z, \frac{1}{4} - y]$ | [181] |
| 182 | $[x, z, y + \frac{1}{2}]$ | [182] |
| 183 | $[\frac{3}{4} - z, y, \frac{1}{4} - x]$ | [183] |
| 184 | $[z, y, x + \frac{1}{2}]$ | [184] |
| 185 | $[\frac{1}{2} - z, \frac{1}{2} - x, -y]$ | [185] |
| 186 | $[\frac{1}{2} - y, \frac{1}{2} - z, -x]$ | [186] |
| 187 | $[y + \frac{3}{4}, \frac{1}{2} - z, x + \frac{1}{4}]$ | [187] |
| 188 | $[z + \frac{3}{4}, x + \frac{3}{4}, -y]$ | [188] |
| 189 | $[y + \frac{3}{4}, z + \frac{3}{4}, -x]$ | [189] |
| 190 | $[\frac{1}{2} - z, x + \frac{3}{4}, y + \frac{1}{4}]$ | [190] |
| 191 | $[\frac{1}{2} - y, z + \frac{3}{4}, x + \frac{1}{4}]$ | [191] |
| 192 | $[z + \frac{3}{4}, \frac{1}{2} - x, y + \frac{1}{4}]$ | [192] |