

Table 1: Wyckoff site: 6a, site symmetry: $-3m$.

| No. | position | mapping |
|-----|---|--|
| 1 | $[0, 0, 0]$ | $[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]$ |
| 2 | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{3}]$ | $[13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24]$ |
| 3 | $[\frac{1}{3}, \frac{2}{3}, \frac{2}{3}]$ | $[25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36]$ |
| 4 | $[0, 0, \frac{1}{2}]$ | $[37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48]$ |
| 5 | $[\frac{2}{3}, \frac{1}{3}, \frac{5}{6}]$ | $[49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60]$ |
| 6 | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{6}]$ | $[61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72]$ |

 Table 2: Wyckoff site: 6b, site symmetry: $-3'm$.

| No. | position | mapping |
|-----|---|--|
| 1 | $[0, 0, \frac{1}{4}]$ | $[1, 2, 3, 10, 11, 12, 40, 41, 42, 43, 44, 45]$ |
| 2 | $[0, 0, \frac{3}{4}]$ | $[4, 5, 6, 7, 8, 9, 37, 38, 39, 46, 47, 48]$ |
| 3 | $[\frac{2}{3}, \frac{1}{3}, \frac{7}{12}]$ | $[13, 14, 15, 22, 23, 24, 52, 53, 54, 55, 56, 57]$ |
| 4 | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{12}]$ | $[16, 17, 18, 19, 20, 21, 49, 50, 51, 58, 59, 60]$ |
| 5 | $[\frac{1}{3}, \frac{2}{3}, \frac{11}{12}]$ | $[25, 26, 27, 34, 35, 36, 64, 65, 66, 67, 68, 69]$ |
| 6 | $[\frac{1}{3}, \frac{2}{3}, \frac{5}{12}]$ | $[28, 29, 30, 31, 32, 33, 61, 62, 63, 70, 71, 72]$ |

 Table 3: Wyckoff site: 12c, site symmetry: $3m$.

| No. | position | mapping |
|-----|---|----------------------------|
| 1 | $[0, 0, z]$ | $[1, 2, 3, 10, 11, 12]$ |
| 2 | $[0, 0, -z]$ | $[4, 5, 6, 7, 8, 9]$ |
| 3 | $[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{3}]$ | $[13, 14, 15, 22, 23, 24]$ |
| 4 | $[\frac{2}{3}, \frac{1}{3}, \frac{1}{3} - z]$ | $[16, 17, 18, 19, 20, 21]$ |
| 5 | $[\frac{1}{3}, \frac{2}{3}, z + \frac{2}{3}]$ | $[25, 26, 27, 34, 35, 36]$ |
| 6 | $[\frac{1}{3}, \frac{2}{3}, \frac{2}{3} - z]$ | $[28, 29, 30, 31, 32, 33]$ |
| 7 | $[0, 0, z + \frac{1}{2}]$ | $[37, 38, 39, 46, 47, 48]$ |
| 8 | $[0, 0, \frac{1}{2} - z]$ | $[40, 41, 42, 43, 44, 45]$ |
| 9 | $[\frac{2}{3}, \frac{1}{3}, z + \frac{5}{6}]$ | $[49, 50, 51, 58, 59, 60]$ |
| 10 | $[\frac{2}{3}, \frac{1}{3}, \frac{5}{6} - z]$ | $[52, 53, 54, 55, 56, 57]$ |
| 11 | $[\frac{1}{3}, \frac{2}{3}, z + \frac{1}{6}]$ | $[61, 62, 63, 70, 71, 72]$ |
| 12 | $[\frac{1}{3}, \frac{2}{3}, \frac{1}{6} - z]$ | $[64, 65, 66, 67, 68, 69]$ |

Table 4: Wyckoff site: 18d, site symmetry: $.2'/m$.

| No. | position | mapping |
|-----|---|------------------|
| 1 | $[\frac{1}{2}, 0, \frac{1}{4}]$ | [1, 10, 40, 43] |
| 2 | $[0, \frac{1}{2}, \frac{1}{4}]$ | [2, 11, 41, 44] |
| 3 | $[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$ | [3, 12, 42, 45] |
| 4 | $[\frac{1}{2}, 0, \frac{3}{4}]$ | [4, 7, 37, 46] |
| 5 | $[0, \frac{1}{2}, \frac{3}{4}]$ | [5, 8, 38, 47] |
| 6 | $[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$ | [6, 9, 39, 48] |
| 7 | $[\frac{1}{6}, \frac{1}{3}, \frac{7}{12}]$ | [13, 22, 52, 55] |
| 8 | $[\frac{2}{3}, \frac{5}{6}, \frac{7}{12}]$ | [14, 23, 53, 56] |
| 9 | $[\frac{1}{6}, \frac{5}{6}, \frac{7}{12}]$ | [15, 24, 54, 57] |
| 10 | $[\frac{1}{6}, \frac{1}{3}, \frac{1}{12}]$ | [16, 19, 49, 58] |
| 11 | $[\frac{2}{3}, \frac{5}{6}, \frac{1}{12}]$ | [17, 20, 50, 59] |
| 12 | $[\frac{1}{6}, \frac{5}{6}, \frac{1}{12}]$ | [18, 21, 51, 60] |
| 13 | $[\frac{5}{6}, \frac{2}{3}, \frac{11}{12}]$ | [25, 34, 64, 67] |
| 14 | $[\frac{1}{3}, \frac{1}{6}, \frac{11}{12}]$ | [26, 35, 65, 68] |
| 15 | $[\frac{5}{6}, \frac{1}{6}, \frac{11}{12}]$ | [27, 36, 66, 69] |
| 16 | $[\frac{5}{6}, \frac{2}{3}, \frac{5}{12}]$ | [28, 31, 61, 70] |
| 17 | $[\frac{1}{3}, \frac{1}{6}, \frac{5}{12}]$ | [29, 32, 62, 71] |
| 18 | $[\frac{5}{6}, \frac{1}{6}, \frac{5}{12}]$ | [30, 33, 63, 72] |

Table 5: Wyckoff site: 18e, site symmetry: $.2/m$.

| No. | position | mapping |
|-----|---|------------------|
| 1 | $[\frac{1}{2}, 0, 0]$ | [1, 4, 7, 10] |
| 2 | $[0, \frac{1}{2}, 0]$ | [2, 5, 8, 11] |
| 3 | $[\frac{1}{2}, \frac{1}{2}, 0]$ | [3, 6, 9, 12] |
| 4 | $[\frac{1}{6}, \frac{1}{3}, \frac{1}{3}]$ | [13, 16, 19, 22] |
| 5 | $[\frac{2}{3}, \frac{5}{6}, \frac{1}{3}]$ | [14, 17, 20, 23] |
| 6 | $[\frac{1}{6}, \frac{5}{6}, \frac{1}{3}]$ | [15, 18, 21, 24] |
| 7 | $[\frac{5}{6}, \frac{2}{3}, \frac{2}{3}]$ | [25, 28, 31, 34] |
| 8 | $[\frac{1}{3}, \frac{1}{6}, \frac{2}{3}]$ | [26, 29, 32, 35] |
| 9 | $[\frac{5}{6}, \frac{1}{6}, \frac{2}{3}]$ | [27, 30, 33, 36] |
| 10 | $[\frac{1}{2}, 0, \frac{1}{2}]$ | [37, 40, 43, 46] |
| 11 | $[0, \frac{1}{2}, \frac{1}{2}]$ | [38, 41, 44, 47] |
| 12 | $[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$ | [39, 42, 45, 48] |
| 13 | $[\frac{1}{6}, \frac{1}{3}, \frac{5}{6}]$ | [49, 52, 55, 58] |
| 14 | $[\frac{2}{3}, \frac{5}{6}, \frac{5}{6}]$ | [50, 53, 56, 59] |
| 15 | $[\frac{1}{6}, \frac{5}{6}, \frac{5}{6}]$ | [51, 54, 57, 60] |
| 16 | $[\frac{5}{6}, \frac{2}{3}, \frac{1}{6}]$ | [61, 64, 67, 70] |
| 17 | $[\frac{1}{3}, \frac{1}{6}, \frac{1}{6}]$ | [62, 65, 68, 71] |
| 18 | $[\frac{5}{6}, \frac{1}{6}, \frac{1}{6}]$ | [63, 66, 69, 72] |

Table 6: Wyckoff site: $36f$, site symmetry: $.2$.

| No. | position | mapping |
|-----|---|---------|
| 1 | $[x, 0, 0]$ | [1,4] |
| 2 | $[0, x, 0]$ | [2,5] |
| 3 | $[-x, -x, 0]$ | [3,6] |
| 4 | $[-x, 0, 0]$ | [7,10] |
| 5 | $[0, -x, 0]$ | [8,11] |
| 6 | $[x, x, 0]$ | [9,12] |
| 7 | $[x + \frac{2}{3}, \frac{1}{3}, \frac{1}{3}]$ | [13,16] |
| 8 | $[\frac{2}{3}, x + \frac{1}{3}, \frac{1}{3}]$ | [14,17] |
| 9 | $[\frac{2}{3} - x, \frac{1}{3} - x, \frac{1}{3}]$ | [15,18] |
| 10 | $[\frac{2}{3} - x, \frac{1}{3}, \frac{1}{3}]$ | [19,22] |
| 11 | $[\frac{2}{3}, \frac{1}{3} - x, \frac{1}{3}]$ | [20,23] |
| 12 | $[x + \frac{2}{3}, x + \frac{1}{3}, \frac{1}{3}]$ | [21,24] |
| 13 | $[x + \frac{1}{3}, \frac{2}{3}, \frac{2}{3}]$ | [25,28] |
| 14 | $[\frac{1}{3}, x + \frac{2}{3}, \frac{2}{3}]$ | [26,29] |
| 15 | $[\frac{1}{3} - x, \frac{2}{3} - x, \frac{2}{3}]$ | [27,30] |
| 16 | $[\frac{1}{3} - x, \frac{2}{3}, \frac{2}{3}]$ | [31,34] |
| 17 | $[\frac{1}{3}, \frac{2}{3} - x, \frac{2}{3}]$ | [32,35] |
| 18 | $[x + \frac{1}{3}, x + \frac{2}{3}, \frac{2}{3}]$ | [33,36] |
| 19 | $[x, 0, \frac{1}{2}]$ | [37,40] |
| 20 | $[0, x, \frac{1}{2}]$ | [38,41] |
| 21 | $[-x, -x, \frac{1}{2}]$ | [39,42] |
| 22 | $[-x, 0, \frac{1}{2}]$ | [43,46] |
| 23 | $[0, -x, \frac{1}{2}]$ | [44,47] |
| 24 | $[x, x, \frac{1}{2}]$ | [45,48] |
| 25 | $[x + \frac{2}{3}, \frac{1}{3}, \frac{5}{6}]$ | [49,52] |
| 26 | $[\frac{2}{3}, x + \frac{1}{3}, \frac{5}{6}]$ | [50,53] |
| 27 | $[\frac{2}{3} - x, \frac{1}{3} - x, \frac{5}{6}]$ | [51,54] |
| 28 | $[\frac{2}{3} - x, \frac{1}{3}, \frac{5}{6}]$ | [55,58] |
| 29 | $[\frac{2}{3}, \frac{1}{3} - x, \frac{5}{6}]$ | [56,59] |
| 30 | $[x + \frac{2}{3}, x + \frac{1}{3}, \frac{5}{6}]$ | [57,60] |
| 31 | $[x + \frac{1}{3}, \frac{2}{3}, \frac{1}{6}]$ | [61,64] |
| 32 | $[\frac{1}{3}, x + \frac{2}{3}, \frac{1}{6}]$ | [62,65] |
| 33 | $[\frac{1}{3} - x, \frac{2}{3} - x, \frac{1}{6}]$ | [63,66] |
| 34 | $[\frac{1}{3} - x, \frac{2}{3}, \frac{1}{6}]$ | [67,70] |
| 35 | $[\frac{1}{3}, \frac{2}{3} - x, \frac{1}{6}]$ | [68,71] |
| 36 | $[x + \frac{1}{3}, x + \frac{2}{3}, \frac{1}{6}]$ | [69,72] |

Table 7: Wyckoff site: $36g$, site symmetry: $.2'$.

| No. | position | mapping |
|-----|-------------------------|---------|
| 1 | $[x, 0, \frac{1}{4}]$ | [1,40] |
| 2 | $[0, x, \frac{1}{4}]$ | [2,41] |
| 3 | $[-x, -x, \frac{1}{4}]$ | [3,42] |

continued ...

Table 7

| No. | position | mapping |
|-----|---|----------|
| 4 | $[x, 0, \frac{3}{4}]$ | [4, 37] |
| 5 | $[0, x, \frac{3}{4}]$ | [5, 38] |
| 6 | $[-x, -x, \frac{3}{4}]$ | [6, 39] |
| 7 | $[-x, 0, \frac{3}{4}]$ | [7, 46] |
| 8 | $[0, -x, \frac{3}{4}]$ | [8, 47] |
| 9 | $[x, x, \frac{3}{4}]$ | [9, 48] |
| 10 | $[-x, 0, \frac{1}{4}]$ | [10, 43] |
| 11 | $[0, -x, \frac{1}{4}]$ | [11, 44] |
| 12 | $[x, x, \frac{1}{4}]$ | [12, 45] |
| 13 | $[x + \frac{2}{3}, \frac{1}{3}, \frac{7}{12}]$ | [13, 52] |
| 14 | $[\frac{2}{3}, x + \frac{1}{3}, \frac{7}{12}]$ | [14, 53] |
| 15 | $[\frac{2}{3} - x, \frac{1}{3} - x, \frac{7}{12}]$ | [15, 54] |
| 16 | $[x + \frac{2}{3}, \frac{1}{3}, \frac{1}{12}]$ | [16, 49] |
| 17 | $[\frac{2}{3}, x + \frac{1}{3}, \frac{1}{12}]$ | [17, 50] |
| 18 | $[\frac{2}{3} - x, \frac{1}{3} - x, \frac{1}{12}]$ | [18, 51] |
| 19 | $[\frac{2}{3} - x, \frac{1}{3}, \frac{1}{12}]$ | [19, 58] |
| 20 | $[\frac{2}{3}, \frac{1}{3} - x, \frac{1}{12}]$ | [20, 59] |
| 21 | $[x + \frac{2}{3}, x + \frac{1}{3}, \frac{1}{12}]$ | [21, 60] |
| 22 | $[\frac{2}{3} - x, \frac{1}{3}, \frac{7}{12}]$ | [22, 55] |
| 23 | $[\frac{2}{3}, \frac{1}{3} - x, \frac{7}{12}]$ | [23, 56] |
| 24 | $[x + \frac{2}{3}, x + \frac{1}{3}, \frac{7}{12}]$ | [24, 57] |
| 25 | $[x + \frac{1}{3}, \frac{2}{3}, \frac{11}{12}]$ | [25, 64] |
| 26 | $[\frac{1}{3}, x + \frac{2}{3}, \frac{11}{12}]$ | [26, 65] |
| 27 | $[\frac{1}{3} - x, \frac{2}{3} - x, \frac{11}{12}]$ | [27, 66] |
| 28 | $[x + \frac{1}{3}, \frac{2}{3}, \frac{5}{12}]$ | [28, 61] |
| 29 | $[\frac{1}{3}, x + \frac{2}{3}, \frac{5}{12}]$ | [29, 62] |
| 30 | $[\frac{1}{3} - x, \frac{2}{3} - x, \frac{5}{12}]$ | [30, 63] |
| 31 | $[\frac{1}{3} - x, \frac{2}{3}, \frac{5}{12}]$ | [31, 70] |
| 32 | $[\frac{1}{3}, \frac{2}{3} - x, \frac{5}{12}]$ | [32, 71] |
| 33 | $[x + \frac{1}{3}, x + \frac{2}{3}, \frac{5}{12}]$ | [33, 72] |
| 34 | $[\frac{1}{3} - x, \frac{2}{3}, \frac{11}{12}]$ | [34, 67] |
| 35 | $[\frac{1}{3}, \frac{2}{3} - x, \frac{11}{12}]$ | [35, 68] |
| 36 | $[x + \frac{1}{3}, x + \frac{2}{3}, \frac{11}{12}]$ | [36, 69] |

Table 8: Wyckoff site: 36h, site symmetry: .m.

| No. | position | mapping |
|-----|---|----------|
| 1 | $[x, -x, z]$ | [1, 11] |
| 2 | $[x, 2x, z]$ | [2, 12] |
| 3 | $[-2x, -x, z]$ | [3, 10] |
| 4 | $[2x, x, -z]$ | [4, 9] |
| 5 | $[-x, x, -z]$ | [5, 7] |
| 6 | $[-x, -2x, -z]$ | [6, 8] |
| 7 | $[x + \frac{2}{3}, \frac{1}{3} - x, z + \frac{1}{3}]$ | [13, 23] |

continued ...

Table 8

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

Table 9: Wyckoff site: 72i, site symmetry: 1

| No. | position | mapping |
|-----|--------------------|---------|
| 1 | $[x, y, z]$ | [1] |
| 2 | $[-y, x - y, z]$ | [2] |
| 3 | $[-x + y, -x, z]$ | [3] |
| 4 | $[x - y, -y, -z]$ | [4] |
| 5 | $[y, x, -z]$ | [5] |
| 6 | $[-x, -x + y, -z]$ | [6] |
| 7 | $[-x, -y, -z]$ | [7] |
| 8 | $[y, -x + y, -z]$ | [8] |
| 9 | $[x - y, x, -z]$ | [9] |
| 10 | $[-x + y, y, z]$ | [10] |
| 11 | $[-y, -x, z]$ | [11] |

continued ...

Table 9

| No. | position | mapping |
|-----|--|---------|
| 12 | $[x, x - y, z]$ | [12] |
| 13 | $[x + \frac{2}{3}, y + \frac{1}{3}, z + \frac{1}{3}]$ | [13] |
| 14 | $[\frac{2}{3} - y, x - y + \frac{1}{3}, z + \frac{1}{3}]$ | [14] |
| 15 | $[-x + y + \frac{2}{3}, \frac{1}{3} - x, z + \frac{1}{3}]$ | [15] |
| 16 | $[x - y + \frac{2}{3}, \frac{1}{3} - y, \frac{1}{3} - z]$ | [16] |
| 17 | $[y + \frac{2}{3}, x + \frac{1}{3}, \frac{1}{3} - z]$ | [17] |
| 18 | $[\frac{2}{3} - x, -x + y + \frac{1}{3}, \frac{1}{3} - z]$ | [18] |
| 19 | $[\frac{2}{3} - x, \frac{1}{3} - y, \frac{1}{3} - z]$ | [19] |
| 20 | $[y + \frac{2}{3}, -x + y + \frac{1}{3}, \frac{1}{3} - z]$ | [20] |
| 21 | $[x - y + \frac{2}{3}, x + \frac{1}{3}, \frac{1}{3} - z]$ | [21] |
| 22 | $[-x + y + \frac{2}{3}, y + \frac{1}{3}, z + \frac{1}{3}]$ | [22] |
| 23 | $[\frac{2}{3} - y, \frac{1}{3} - x, z + \frac{1}{3}]$ | [23] |
| 24 | $[x + \frac{2}{3}, x - y + \frac{1}{3}, z + \frac{1}{3}]$ | [24] |
| 25 | $[x + \frac{1}{3}, y + \frac{2}{3}, z + \frac{2}{3}]$ | [25] |
| 26 | $[\frac{1}{3} - y, x - y + \frac{2}{3}, z + \frac{2}{3}]$ | [26] |
| 27 | $[-x + y + \frac{1}{3}, \frac{2}{3} - x, z + \frac{2}{3}]$ | [27] |
| 28 | $[x - y + \frac{1}{3}, \frac{2}{3} - y, \frac{2}{3} - z]$ | [28] |
| 29 | $[y + \frac{1}{3}, x + \frac{2}{3}, \frac{2}{3} - z]$ | [29] |
| 30 | $[\frac{1}{3} - x, -x + y + \frac{2}{3}, \frac{2}{3} - z]$ | [30] |
| 31 | $[\frac{1}{3} - x, \frac{2}{3} - y, \frac{2}{3} - z]$ | [31] |
| 32 | $[y + \frac{1}{3}, -x + y + \frac{2}{3}, \frac{2}{3} - z]$ | [32] |
| 33 | $[x - y + \frac{1}{3}, x + \frac{2}{3}, \frac{2}{3} - z]$ | [33] |
| 34 | $[-x + y + \frac{1}{3}, y + \frac{2}{3}, z + \frac{2}{3}]$ | [34] |
| 35 | $[\frac{1}{3} - y, \frac{2}{3} - x, z + \frac{2}{3}]$ | [35] |
| 36 | $[x + \frac{1}{3}, x - y + \frac{2}{3}, z + \frac{2}{3}]$ | [36] |
| 37 | $[x, y, z + \frac{1}{2}]$ | [37] |
| 38 | $[-y, x - y, z + \frac{1}{2}]$ | [38] |
| 39 | $[-x + y, -x, z + \frac{1}{2}]$ | [39] |
| 40 | $[x - y, -y, \frac{1}{2} - z]$ | [40] |
| 41 | $[y, x, \frac{1}{2} - z]$ | [41] |
| 42 | $[-x, -x + y, \frac{1}{2} - z]$ | [42] |
| 43 | $[-x, -y, \frac{1}{2} - z]$ | [43] |
| 44 | $[y, -x + y, \frac{1}{2} - z]$ | [44] |
| 45 | $[x - y, x, \frac{1}{2} - z]$ | [45] |
| 46 | $[-x + y, y, z + \frac{1}{2}]$ | [46] |
| 47 | $[-y, -x, z + \frac{1}{2}]$ | [47] |
| 48 | $[x, x - y, z + \frac{1}{2}]$ | [48] |
| 49 | $[x + \frac{2}{3}, y + \frac{1}{3}, z + \frac{5}{6}]$ | [49] |
| 50 | $[\frac{2}{3} - y, x - y + \frac{1}{3}, z + \frac{5}{6}]$ | [50] |
| 51 | $[-x + y + \frac{2}{3}, \frac{1}{3} - x, z + \frac{5}{6}]$ | [51] |
| 52 | $[x - y + \frac{2}{3}, \frac{1}{3} - y, \frac{5}{6} - z]$ | [52] |
| 53 | $[y + \frac{2}{3}, x + \frac{1}{3}, \frac{5}{6} - z]$ | [53] |
| 54 | $[\frac{2}{3} - x, -x + y + \frac{1}{3}, \frac{5}{6} - z]$ | [54] |
| 55 | $[\frac{2}{3} - x, \frac{1}{3} - y, \frac{5}{6} - z]$ | [55] |
| 56 | $[y + \frac{2}{3}, -x + y + \frac{1}{3}, \frac{5}{6} - z]$ | [56] |
| 57 | $[x - y + \frac{2}{3}, x + \frac{1}{3}, \frac{5}{6} - z]$ | [57] |
| 58 | $[-x + y + \frac{2}{3}, y + \frac{1}{3}, z + \frac{5}{6}]$ | [58] |

continued ...

Table 9

| No. | position | mapping |
|-----|--|---------|
| 59 | $[\frac{2}{3} - y, \frac{1}{3} - x, z + \frac{5}{6}]$ | [59] |
| 60 | $[x + \frac{2}{3}, x - y + \frac{1}{3}, z + \frac{5}{6}]$ | [60] |
| 61 | $[x + \frac{1}{3}, y + \frac{2}{3}, z + \frac{1}{6}]$ | [61] |
| 62 | $[\frac{1}{3} - y, x - y + \frac{2}{3}, z + \frac{1}{6}]$ | [62] |
| 63 | $[-x + y + \frac{1}{3}, \frac{2}{3} - x, z + \frac{1}{6}]$ | [63] |
| 64 | $[x - y + \frac{1}{3}, \frac{2}{3} - y, \frac{1}{6} - z]$ | [64] |
| 65 | $[y + \frac{1}{3}, x + \frac{2}{3}, \frac{1}{6} - z]$ | [65] |
| 66 | $[\frac{1}{3} - x, -x + y + \frac{2}{3}, \frac{1}{6} - z]$ | [66] |
| 67 | $[\frac{1}{3} - x, \frac{2}{3} - y, \frac{1}{6} - z]$ | [67] |
| 68 | $[y + \frac{1}{3}, -x + y + \frac{2}{3}, \frac{1}{6} - z]$ | [68] |
| 69 | $[x - y + \frac{1}{3}, x + \frac{2}{3}, \frac{1}{6} - z]$ | [69] |
| 70 | $[-x + y + \frac{1}{3}, y + \frac{2}{3}, z + \frac{1}{6}]$ | [70] |
| 71 | $[\frac{1}{3} - y, \frac{2}{3} - x, z + \frac{1}{6}]$ | [71] |
| 72 | $[x + \frac{1}{3}, x - y + \frac{2}{3}, z + \frac{1}{6}]$ | [72] |