# MSG No. 67.509  $C_amma$   [ Type IV, orthorhombic ]

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

| No. | position | mapping |
|---|---|---|
| 1 | $\left[0, \frac{1}{4}, 0\right]$ | [1,6,12,15,19,24,26,29] |
| 2 | $\left[0, \frac{3}{4}, 0\right]$ | [2,5,11,16,20,23,25,30] |
| 3 | $\left[\frac{1}{2}, \frac{1}{4}, 0\right]$ | [3,8,10,13,17,22,28,31] |
| 4 | $\left[\frac{1}{2}, \frac{3}{4}, 0\right]$ | [4,7,9,14,18,21,27,32] |

Table 2: Wyckoff site: 4b, site symmetry: mm'm'

| No. | position | mapping |
|---|---|---|
| 1 | $[0, 0, 0]$ | [1,2,5,6,19,20,23,24] |
| 2 | $\left[\frac{1}{2}, 0, 0\right]$ | [3,4,7,8,17,18,21,22] |
| 3 | $\left[\frac{1}{2}, \frac{1}{2}, 0\right]$ | [9,10,13,14,27,28,31,32] |
| 4 | $\left[0, \frac{1}{2}, 0\right]$ | [11,12,15,16,25,26,29,30] |

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

| No. | position | mapping |
|---|---|---|
| 1 | $\left[0, \frac{1}{4}, \frac{1}{2}\right]$ | [1,6,12,15,19,24,26,29] |
| 2 | $\left[0, \frac{3}{4}, \frac{1}{2}\right]$ | [2,5,11,16,20,23,25,30] |
| 3 | $\left[\frac{1}{2}, \frac{1}{4}, \frac{1}{2}\right]$ | [3,8,10,13,17,22,28,31] |
| 4 | $\left[\frac{1}{2}, \frac{3}{4}, \frac{1}{2}\right]$ | [4,7,9,14,18,21,27,32] |

Table 4: Wyckoff site: 4d, site symmetry: mm'm'

| No. | position | mapping |
|---|---|---|
| 1 | $\left[0, 0, \frac{1}{2}\right]$ | [1,2,5,6,19,20,23,24] |
| 2 | $\left[\frac{1}{2}, 0, \frac{1}{2}\right]$ | [3,4,7,8,17,18,21,22] |
| 3 | $\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$ | [9,10,13,14,27,28,31,32] |
| 4 | $\left[0, \frac{1}{2}, \frac{1}{2}\right]$ | [11,12,15,16,25,26,29,30] |

Table 5: Wyckoff site: 4e, site symmetry: m'mm'

| No. | position | mapping |
|---|---|---|
| 1 | $\left[\frac{1}{4}, \frac{1}{4}, 0\right]$ | [1,3,13,15,22,24,26,28] |
| 2 | $\left[\frac{1}{4}, \frac{3}{4}, 0\right]$ | [2,4,14,16,21,23,25,27] |

*continued ...*

Table 5

| No. | position | mapping |
|---|---|---|
| 3 | $\left[\frac{3}{4}, \frac{3}{4}, 0\right]$ | [5,7,9,11,18,20,30,32] |
| 4 | $\left[\frac{3}{4}, \frac{1}{4}, 0\right]$ | [6,8,10,12,17,19,29,31] |

Table 6: Wyckoff site: 4f, site symmetry: m'm'm'

| No. | position | mapping |
|---|---|---|
| 1 | $\left[\frac{1}{4}, 0, 0\right]$ | [1,2,3,4,21,22,23,24] |
| 2 | $\left[\frac{3}{4}, 0, 0\right]$ | [5,6,7,8,17,18,19,20] |
| 3 | $\left[\frac{3}{4}, \frac{1}{2}, 0\right]$ | [9,10,11,12,29,30,31,32] |
| 4 | $\left[\frac{1}{4}, \frac{1}{2}, 0\right]$ | [13,14,15,16,25,26,27,28] |

Table 7: Wyckoff site: 4g, site symmetry: m'mm'

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

Table 8: Wyckoff site: 4h, site symmetry: m'm'm'

| No. | position | mapping |
|---|---|---|
| 1 | $\left[\frac{1}{4}, 0, \frac{1}{2}\right]$ | [1,2,3,4,21,22,23,24] |
| 2 | $\left[\frac{3}{4}, 0, \frac{1}{2}\right]$ | [5,6,7,8,17,18,19,20] |
| 3 | $\left[\frac{3}{4}, \frac{1}{2}, \frac{1}{2}\right]$ | [9,10,11,12,29,30,31,32] |
| 4 | $\left[\frac{1}{4}, \frac{1}{2}, \frac{1}{2}\right]$ | [13,14,15,16,25,26,27,28] |

Table 9: Wyckoff site: 8i, site symmetry: m2'm'

| No. | position | mapping |
|---|---|---|
| 1 | $[0, y, 0]$ | [1,6,19,24] |
| 2 | $[0, -y, 0]$ | [2,5,20,23] |
| 3 | $\left[\frac{1}{2}, y, 0\right]$ | [3,8,17,22] |
| 4 | $\left[\frac{1}{2}, -y, 0\right]$ | [4,7,18,21] |
| 5 | $\left[\frac{1}{2}, y + \frac{1}{2}, 0\right]$ | [9,14,27,32] |
| 6 | $\left[\frac{1}{2}, \frac{1}{2} - y, 0\right]$ | [10,13,28,31] |
| 7 | $\left[0, y + \frac{1}{2}, 0\right]$ | [11,16,25,30] |

Table 9

| No. | position | mapping |
|-----|----------|---------|
| 8 | $\left[0, \frac{1}{2} - y, 0\right]$ | [12,15,26,29] |

Table 10: Wyckoff site: 8j, site symmetry: m2'm'

| No. | position | mapping |
|-----|----------|---------|
| 1 | $\left[0, y, \frac{1}{2}\right]$ | [1,6,19,24] |
| 2 | $\left[0, -y, \frac{1}{2}\right]$ | [2,5,20,23] |
| 3 | $\left[\frac{1}{2}, y, \frac{1}{2}\right]$ | [3,8,17,22] |
| 4 | $\left[\frac{1}{2}, -y, \frac{1}{2}\right]$ | [4,7,18,21] |
| 5 | $\left[\frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}\right]$ | [9,14,27,32] |
| 6 | $\left[\frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}\right]$ | [10,13,28,31] |
| 7 | $\left[0, y + \frac{1}{2}, \frac{1}{2}\right]$ | [11,16,25,30] |
| 8 | $\left[0, \frac{1}{2} - y, \frac{1}{2}\right]$ | [12,15,26,29] |

Table 11: Wyckoff site: 8k, site symmetry: m'2m'

| No. | position | mapping |
|-----|----------|---------|
| 1 | $\left[\frac{1}{4}, y, 0\right]$ | [1,3,22,24] |
| 2 | $\left[\frac{1}{4}, -y, 0\right]$ | [2,4,21,23] |
| 3 | $\left[\frac{3}{4}, -y, 0\right]$ | [5,7,18,20] |
| 4 | $\left[\frac{3}{4}, y, 0\right]$ | [6,8,17,19] |
| 5 | $\left[\frac{3}{4}, y + \frac{1}{2}, 0\right]$ | [9,11,30,32] |
| 6 | $\left[\frac{3}{4}, \frac{1}{2} - y, 0\right]$ | [10,12,29,31] |
| 7 | $\left[\frac{1}{4}, \frac{1}{2} - y, 0\right]$ | [13,15,26,28] |
| 8 | $\left[\frac{1}{4}, y + \frac{1}{2}, 0\right]$ | [14,16,25,27] |

Table 12: Wyckoff site: 8l, site symmetry: m'2m'

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

Table 13: Wyckoff site: 8m, site symmetry: 2'mm'

| No. | position | mapping |
|-----|----------|---------|
| 1 | $\left[x, \frac{1}{4}, 0\right]$ | [1,15,24,26] |
| 2 | $\left[x, \frac{3}{4}, 0\right]$ | [2,16,23,25] |
| 3 | $\left[\frac{1}{2} - x, \frac{1}{4}, 0\right]$ | [3,13,22,28] |
| 4 | $\left[\frac{1}{2} - x, \frac{3}{4}, 0\right]$ | [4,14,21,27] |
| 5 | $\left[-x, \frac{3}{4}, 0\right]$ | [5,11,20,30] |
| 6 | $\left[-x, \frac{1}{4}, 0\right]$ | [6,12,19,29] |
| 7 | $\left[x + \frac{1}{2}, \frac{3}{4}, 0\right]$ | [7,9,18,32] |
| 8 | $\left[x + \frac{1}{2}, \frac{1}{4}, 0\right]$ | [8,10,17,31] |

Table 14: Wyckoff site: 8n, site symmetry: 2'mm'

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

Table 15: Wyckoff site: 8o, site symmetry: 2m'm'

| No. | position | mapping |
|-----|----------|---------|
| 1 | $[x, 0, 0]$ | [1,2,23,24] |
| 2 | $\left[\frac{1}{2} - x, 0, 0\right]$ | [3,4,21,22] |
| 3 | $[-x, 0, 0]$ | [5,6,19,20] |
| 4 | $\left[x + \frac{1}{2}, 0, 0\right]$ | [7,8,17,18] |
| 5 | $\left[x + \frac{1}{2}, \frac{1}{2}, 0\right]$ | [9,10,31,32] |
| 6 | $\left[-x, \frac{1}{2}, 0\right]$ | [11,12,29,30] |
| 7 | $\left[\frac{1}{2} - x, \frac{1}{2}, 0\right]$ | [13,14,27,28] |
| 8 | $\left[x, \frac{1}{2}, 0\right]$ | [15,16,25,26] |

Table 16: Wyckoff site: 8p, site symmetry: 2m'm'

| No. | position | mapping |
|-----|----------|---------|
| 1 | $\left[x, 0, \frac{1}{2}\right]$ | [1,2,23,24] |
| 2 | $\left[\frac{1}{2} - x, 0, \frac{1}{2}\right]$ | [3,4,21,22] |
| 3 | $\left[-x, 0, \frac{1}{2}\right]$ | [5,6,19,20] |

*continued ...*

Table 16

| No. | position | mapping |
|-----|----------|---------|
| 4 | $\left[x+\frac{1}{2}, 0, \frac{1}{2}\right]$ | [7,8,17,18] |
| 5 | $\left[x+\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$ | [9,10,31,32] |
| 6 | $\left[-x, \frac{1}{2}, \frac{1}{2}\right]$ | [11,12,29,30] |
| 7 | $\left[\frac{1}{2}-x, \frac{1}{2}, \frac{1}{2}\right]$ | [13,14,27,28] |
| 8 | $\left[x, \frac{1}{2}, \frac{1}{2}\right]$ | [15,16,25,26] |

Table 17: Wyckoff site: `8q`, site symmetry: `mm2`

| No. | position | mapping |
|-----|----------|---------|
| 1 | $\left[0, \frac{1}{4}, z\right]$ | [1,6,12,15] |
| 2 | $\left[0, \frac{3}{4}, -z\right]$ | [2,5,11,16] |
| 3 | $\left[\frac{1}{2}, \frac{1}{4}, -z\right]$ | [3,8,10,13] |
| 4 | $\left[\frac{1}{2}, \frac{3}{4}, z\right]$ | [4,7,9,14] |
| 5 | $\left[\frac{1}{2}, \frac{1}{4}, z\right]$ | [17,22,28,31] |
| 6 | $\left[\frac{1}{2}, \frac{3}{4}, -z\right]$ | [18,21,27,32] |
| 7 | $\left[0, \frac{1}{4}, -z\right]$ | [19,24,26,29] |
| 8 | $\left[0, \frac{3}{4}, z\right]$ | [20,23,25,30] |

Table 18: Wyckoff site: `8r`, site symmetry: `m'm2'`

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

Table 19: Wyckoff site: `8s`, site symmetry: `mm'2'`

| No. | position | mapping |
|-----|----------|---------|
| 1 | $[0, 0, z]$ | [1,6,20,23] |
| 2 | $[0, 0, -z]$ | [2,5,19,24] |
| 3 | $\left[\frac{1}{2}, 0, -z\right]$ | [3,8,18,21] |
| 4 | $\left[\frac{1}{2}, 0, z\right]$ | [4,7,17,22] |
| 5 | $\left[\frac{1}{2}, \frac{1}{2}, z\right]$ | [9,14,28,31] |
| 6 | $\left[\frac{1}{2}, \frac{1}{2}, -z\right]$ | [10,13,27,32] |

*continued ...*

Table 19

| No. | position | mapping |
|-----|----------|---------|
| 7 | $\left[0, \frac{1}{2}, -z\right]$ | [11,16,26,29] |
| 8 | $\left[0, \frac{1}{2}, z\right]$ | [12,15,25,30] |

Table 20: Wyckoff site: 8t, site symmetry: m'm'2

| No. | position | mapping |
|-----|----------|---------|
| 1 | $\left[\frac{1}{4}, 0, z\right]$ | [1,4,22,23] |
| 2 | $\left[\frac{1}{4}, 0, -z\right]$ | [2,3,21,24] |
| 3 | $\left[\frac{3}{4}, 0, -z\right]$ | [5,8,18,19] |
| 4 | $\left[\frac{3}{4}, 0, z\right]$ | [6,7,17,20] |
| 5 | $\left[\frac{3}{4}, \frac{1}{2}, z\right]$ | [9,12,30,31] |
| 6 | $\left[\frac{3}{4}, \frac{1}{2}, -z\right]$ | [10,11,29,32] |
| 7 | $\left[\frac{1}{4}, \frac{1}{2}, -z\right]$ | [13,16,26,27] |
| 8 | $\left[\frac{1}{4}, \frac{1}{2}, z\right]$ | [14,15,25,28] |

Table 21: Wyckoff site: 16u, site symmetry: .m.

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

Table 22: Wyckoff site: 16v, site symmetry: .m'.

| No. | position | mapping |
|-----|----------|---------|
| 1 | $[x, 0, z]$ | [1,23] |

Table 22

| No. | position | mapping |
| --- | --- | --- |
| 2 | $[x, 0, -z]$ | [2,24] |
| 3 | $\left[\frac{1}{2} - x, 0, -z\right]$ | [3,21] |
| 4 | $\left[\frac{1}{2} - x, 0, z\right]$ | [4,22] |
| 5 | $[-x, 0, -z]$ | [5,19] |
| 6 | $[-x, 0, z]$ | [6,20] |
| 7 | $\left[x + \frac{1}{2}, 0, z\right]$ | [7,17] |
| 8 | $\left[x + \frac{1}{2}, 0, -z\right]$ | [8,18] |
| 9 | $\left[x + \frac{1}{2}, \frac{1}{2}, z\right]$ | [9,31] |
| 10 | $\left[x + \frac{1}{2}, \frac{1}{2}, -z\right]$ | [10,32] |
| 11 | $\left[-x, \frac{1}{2}, -z\right]$ | [11,29] |
| 12 | $\left[-x, \frac{1}{2}, z\right]$ | [12,30] |
| 13 | $\left[\frac{1}{2} - x, \frac{1}{2}, -z\right]$ | [13,27] |
| 14 | $\left[\frac{1}{2} - x, \frac{1}{2}, z\right]$ | [14,28] |
| 15 | $\left[x, \frac{1}{2}, z\right]$ | [15,25] |
| 16 | $\left[x, \frac{1}{2}, -z\right]$ | [16,26] |

Table 23: Wyckoff site: 16w, site symmetry: m..

| No. | position | mapping |
| --- | --- | --- |
| 1 | $[0, y, z]$ | [1,6] |
| 2 | $[0, -y, -z]$ | [2,5] |
| 3 | $\left[\frac{1}{2}, y, -z\right]$ | [3,8] |
| 4 | $\left[\frac{1}{2}, -y, z\right]$ | [4,7] |
| 5 | $\left[\frac{1}{2}, y + \frac{1}{2}, z\right]$ | [9,14] |
| 6 | $\left[\frac{1}{2}, \frac{1}{2} - y, -z\right]$ | [10,13] |
| 7 | $\left[0, y + \frac{1}{2}, -z\right]$ | [11,16] |
| 8 | $\left[0, \frac{1}{2} - y, z\right]$ | [12,15] |
| 9 | $\left[\frac{1}{2}, y, z\right]$ | [17,22] |
| 10 | $\left[\frac{1}{2}, -y, -z\right]$ | [18,21] |
| 11 | $[0, y, -z]$ | [19,24] |
| 12 | $[0, -y, z]$ | [20,23] |
| 13 | $\left[0, y + \frac{1}{2}, z\right]$ | [25,30] |
| 14 | $\left[0, \frac{1}{2} - y, -z\right]$ | [26,29] |
| 15 | $\left[\frac{1}{2}, y + \frac{1}{2}, -z\right]$ | [27,32] |
| 16 | $\left[\frac{1}{2}, \frac{1}{2} - y, z\right]$ | [28,31] |

Table 24: Wyckoff site: 16x, site symmetry: m'..

| No. | position | mapping |
| --- | --- | --- |
| 1 | $\left[\frac{1}{4}, y, z\right]$ | [1,22] |
| 2 | $\left[\frac{1}{4}, -y, -z\right]$ | [2,21] |
| 3 | $\left[\frac{1}{4}, y, -z\right]$ | [3,24] |

*continued ...*

Table 24

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

Table 25: Wyckoff site: `16y`, site symmetry: `..m'`

| No. | position | mapping |
|-----|----------|---------|
| 1 | $[x, y, 0]$ | [1,24] |
| 2 | $[x, -y, 0]$ | [2,23] |
| 3 | $\left[\frac{1}{2} - x, y, 0\right]$ | [3,22] |
| 4 | $\left[\frac{1}{2} - x, -y, 0\right]$ | [4,21] |
| 5 | $[-x, -y, 0]$ | [5,20] |
| 6 | $[-x, y, 0]$ | [6,19] |
| 7 | $\left[x + \frac{1}{2}, -y, 0\right]$ | [7,18] |
| 8 | $\left[x + \frac{1}{2}, y, 0\right]$ | [8,17] |
| 9 | $\left[x + \frac{1}{2}, y + \frac{1}{2}, 0\right]$ | [9,32] |
| 10 | $\left[x + \frac{1}{2}, \frac{1}{2} - y, 0\right]$ | [10,31] |
| 11 | $\left[-x, y + \frac{1}{2}, 0\right]$ | [11,30] |
| 12 | $\left[-x, \frac{1}{2} - y, 0\right]$ | [12,29] |
| 13 | $\left[\frac{1}{2} - x, \frac{1}{2} - y, 0\right]$ | [13,28] |
| 14 | $\left[\frac{1}{2} - x, y + \frac{1}{2}, 0\right]$ | [14,27] |
| 15 | $\left[x, \frac{1}{2} - y, 0\right]$ | [15,26] |
| 16 | $\left[x, y + \frac{1}{2}, 0\right]$ | [16,25] |

Table 26: Wyckoff site: `16z`, site symmetry: `..m'`

| No. | position | mapping |
|-----|----------|---------|
| 1 | $\left[x, y, \frac{1}{2}\right]$ | [1,24] |
| 2 | $\left[x, -y, \frac{1}{2}\right]$ | [2,23] |
| 3 | $\left[\frac{1}{2} - x, y, \frac{1}{2}\right]$ | [3,22] |
| 4 | $\left[\frac{1}{2} - x, -y, \frac{1}{2}\right]$ | [4,21] |
| 5 | $\left[-x, -y, \frac{1}{2}\right]$ | [5,20] |

*continued ...*

Table 26

| No. | position | mapping |
|-----|----------|---------|
| 6 | $\left[-x,\,y,\,\frac{1}{2}\right]$ | [6,19] |
| 7 | $\left[x+\frac{1}{2},\,-y,\,\frac{1}{2}\right]$ | [7,18] |
| 8 | $\left[x+\frac{1}{2},\,y,\,\frac{1}{2}\right]$ | [8,17] |
| 9 | $\left[x+\frac{1}{2},\,y+\frac{1}{2},\,\frac{1}{2}\right]$ | [9,32] |
| 10 | $\left[x+\frac{1}{2},\,\frac{1}{2}-y,\,\frac{1}{2}\right]$ | [10,31] |
| 11 | $\left[-x,\,y+\frac{1}{2},\,\frac{1}{2}\right]$ | [11,30] |
| 12 | $\left[-x,\,\frac{1}{2}-y,\,\frac{1}{2}\right]$ | [12,29] |
| 13 | $\left[\frac{1}{2}-x,\,\frac{1}{2}-y,\,\frac{1}{2}\right]$ | [13,28] |
| 14 | $\left[\frac{1}{2}-x,\,y+\frac{1}{2},\,\frac{1}{2}\right]$ | [14,27] |
| 15 | $\left[x,\,\frac{1}{2}-y,\,\frac{1}{2}\right]$ | [15,26] |
| 16 | $\left[x,\,y+\frac{1}{2},\,\frac{1}{2}\right]$ | [16,25] |

Table 27: Wyckoff site: `32A`, site symmetry: `1`

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

*continued ...*

Table 27

| No. | position | mapping |
|-----|----------|---------|
| 30 | $\left[-x,\, y + \frac{1}{2},\, z\right]$ | [30] |
| 31 | $\left[x + \frac{1}{2},\, \frac{1}{2} - y,\, z\right]$ | [31] |
| 32 | $\left[x + \frac{1}{2},\, y + \frac{1}{2},\, -z\right]$ | [32] |

| No. | position | mapping |
|-----|----------|---------|
| 30 | $\left[-x,\, y + \frac{1}{2},\, z\right]$ | [30] |
| 31 | $\left[x + \frac{1}{2},\, \frac{1}{2} - y,\, z\right]$ | [31] |
| 32 | $\left[x + \frac{1}{2},\, y + \frac{1}{2},\, -z\right]$ | [32] |