

SG No. 228 $O_h^8 Fd\bar{3}c$ [cubic]

* plus set: $+ [0, 0, 0]$, $+ [0, \frac{1}{2}, \frac{1}{2}]$, $+ [\frac{1}{2}, 0, \frac{1}{2}]$, $+ [\frac{1}{2}, \frac{1}{2}, 0]$

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

| No. | position | mapping |
|-----|---|--|
| 1 | $[\frac{1}{8}, \frac{1}{8}, \frac{1}{8}]$ | [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12] |
| 2 | $[\frac{7}{8}, \frac{3}{8}, \frac{7}{8}]$ | [13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24] |
| 3 | $[\frac{7}{8}, \frac{7}{8}, \frac{7}{8}]$ | [25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36] |
| 4 | $[\frac{1}{8}, \frac{5}{8}, \frac{1}{8}]$ | [37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48] |

Table 2: Wyckoff site: 32b, site symmetry: .32

| No. | position | mapping |
|-----|---|--------------------------|
| 1 | $[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$ | [1, 5, 9, 14, 19, 24] |
| 2 | $[0, \frac{1}{2}, \frac{3}{4}]$ | [2, 7, 12, 13, 17, 21] |
| 3 | $[\frac{1}{2}, \frac{3}{4}, 0]$ | [3, 8, 10, 15, 20, 22] |
| 4 | $[\frac{3}{4}, 0, \frac{1}{2}]$ | [4, 6, 11, 16, 18, 23] |
| 5 | $[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$ | [25, 29, 33, 38, 43, 48] |
| 6 | $[0, \frac{1}{2}, \frac{1}{4}]$ | [26, 31, 36, 37, 41, 45] |
| 7 | $[\frac{1}{2}, \frac{1}{4}, 0]$ | [27, 32, 34, 39, 44, 46] |
| 8 | $[\frac{1}{4}, 0, \frac{1}{2}]$ | [28, 30, 35, 40, 42, 47] |

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

| No. | position | mapping |
|-----|---|--------------------------|
| 1 | [0, 0, 0] | [1, 5, 9, 25, 29, 33] |
| 2 | $[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}]$ | [2, 7, 12, 26, 31, 36] |
| 3 | $[\frac{3}{4}, \frac{1}{2}, \frac{1}{4}]$ | [3, 8, 10, 27, 32, 34] |
| 4 | $[\frac{1}{2}, \frac{1}{4}, \frac{3}{4}]$ | [4, 6, 11, 28, 30, 35] |
| 5 | $[\frac{3}{4}, \frac{1}{4}, 0]$ | [13, 17, 21, 37, 41, 45] |
| 6 | $[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$ | [14, 19, 24, 38, 43, 48] |
| 7 | $[\frac{1}{4}, 0, \frac{3}{4}]$ | [15, 20, 22, 39, 44, 46] |
| 8 | $[0, \frac{3}{4}, \frac{1}{4}]$ | [16, 18, 23, 40, 42, 47] |

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

| No. | position | mapping |
|-----|---|----------------|
| 1 | $[\frac{7}{8}, \frac{1}{8}, \frac{1}{8}]$ | [1, 4, 41, 44] |
| 2 | $[\frac{3}{8}, \frac{5}{8}, \frac{5}{8}]$ | [2, 3, 42, 43] |
| 3 | $[\frac{1}{8}, \frac{7}{8}, \frac{1}{8}]$ | [5, 8, 37, 40] |

continued ...

Table 4

| No. | position | mapping |
|-----|---|------------------|
| 4 | $[\frac{5}{8}, \frac{3}{8}, \frac{5}{8}]$ | [6, 7, 38, 39] |
| 5 | $[\frac{1}{8}, \frac{1}{8}, \frac{7}{8}]$ | [9, 12, 46, 47] |
| 6 | $[\frac{5}{8}, \frac{5}{8}, \frac{3}{8}]$ | [10, 11, 45, 48] |
| 7 | $[\frac{7}{8}, \frac{1}{8}, \frac{7}{8}]$ | [13, 16, 29, 32] |
| 8 | $[\frac{3}{8}, \frac{5}{8}, \frac{3}{8}]$ | [14, 15, 30, 31] |
| 9 | $[\frac{5}{8}, \frac{3}{8}, \frac{7}{8}]$ | [17, 20, 25, 28] |
| 10 | $[\frac{1}{8}, \frac{7}{8}, \frac{3}{8}]$ | [18, 19, 26, 27] |
| 11 | $[\frac{7}{8}, \frac{3}{8}, \frac{1}{8}]$ | [21, 24, 34, 35] |
| 12 | $[\frac{3}{8}, \frac{7}{8}, \frac{5}{8}]$ | [22, 23, 33, 36] |

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

| No. | position | mapping |
|-----|---|--------------|
| 1 | $[x, x, x]$ | [1, 5, 9] |
| 2 | $[\frac{1}{4} - x, \frac{3}{4} - x, x + \frac{1}{2}]$ | [2, 7, 12] |
| 3 | $[\frac{3}{4} - x, x + \frac{1}{2}, \frac{1}{4} - x]$ | [3, 8, 10] |
| 4 | $[x + \frac{1}{2}, \frac{1}{4} - x, \frac{3}{4} - x]$ | [4, 6, 11] |
| 5 | $[x + \frac{3}{4}, x + \frac{1}{4}, -x]$ | [13, 17, 21] |
| 6 | $[\frac{1}{2} - x, \frac{1}{2} - x, \frac{1}{2} - x]$ | [14, 19, 24] |
| 7 | $[x + \frac{1}{4}, -x, x + \frac{3}{4}]$ | [15, 20, 22] |
| 8 | $[-x, x + \frac{3}{4}, x + \frac{1}{4}]$ | [16, 18, 23] |
| 9 | $[-x, -x, -x]$ | [25, 29, 33] |
| 10 | $[x + \frac{3}{4}, x + \frac{1}{4}, \frac{1}{2} - x]$ | [26, 31, 36] |
| 11 | $[x + \frac{1}{4}, \frac{1}{2} - x, x + \frac{3}{4}]$ | [27, 32, 34] |
| 12 | $[\frac{1}{2} - x, x + \frac{3}{4}, x + \frac{1}{4}]$ | [28, 30, 35] |
| 13 | $[\frac{1}{4} - x, \frac{3}{4} - x, x]$ | [37, 41, 45] |
| 14 | $[x + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}]$ | [38, 43, 48] |
| 15 | $[\frac{3}{4} - x, x, \frac{1}{4} - x]$ | [39, 44, 46] |
| 16 | $[x, \frac{1}{4} - x, \frac{3}{4} - x]$ | [40, 42, 47] |

Table 6: Wyckoff site: 96f, site symmetry: $2 \cdot \cdot$

| No. | position | mapping |
|-----|---|----------|
| 1 | $[x, \frac{1}{8}, \frac{1}{8}]$ | [1, 4] |
| 2 | $[\frac{1}{4} - x, \frac{5}{8}, \frac{5}{8}]$ | [2, 3] |
| 3 | $[\frac{1}{8}, x, \frac{1}{8}]$ | [5, 8] |
| 4 | $[\frac{5}{8}, \frac{1}{4} - x, \frac{5}{8}]$ | [6, 7] |
| 5 | $[\frac{1}{8}, \frac{1}{8}, x]$ | [9, 12] |
| 6 | $[\frac{5}{8}, \frac{5}{8}, \frac{1}{4} - x]$ | [10, 11] |
| 7 | $[\frac{7}{8}, x + \frac{1}{4}, \frac{7}{8}]$ | [13, 16] |
| 8 | $[\frac{3}{8}, \frac{1}{2} - x, \frac{3}{8}]$ | [14, 15] |
| 9 | $[x + \frac{3}{4}, \frac{3}{8}, \frac{7}{8}]$ | [17, 20] |

continued ...

Table 6

| No. | position | mapping |
|-----|---|----------|
| 10 | $[-x, \frac{7}{8}, \frac{3}{8}]$ | [18, 19] |
| 11 | $[\frac{7}{8}, \frac{3}{8}, -x]$ | [21, 24] |
| 12 | $[\frac{3}{8}, \frac{7}{8}, x + \frac{3}{4}]$ | [22, 23] |
| 13 | $[-x, \frac{7}{8}, \frac{7}{8}]$ | [25, 28] |
| 14 | $[x + \frac{3}{4}, \frac{3}{8}, \frac{3}{8}]$ | [26, 27] |
| 15 | $[\frac{7}{8}, -x, \frac{7}{8}]$ | [29, 32] |
| 16 | $[\frac{3}{8}, x + \frac{3}{4}, \frac{3}{8}]$ | [30, 31] |
| 17 | $[\frac{7}{8}, \frac{7}{8}, -x]$ | [33, 36] |
| 18 | $[\frac{3}{8}, \frac{3}{8}, x + \frac{3}{4}]$ | [34, 35] |
| 19 | $[\frac{1}{8}, \frac{3}{4} - x, \frac{1}{8}]$ | [37, 40] |
| 20 | $[\frac{5}{8}, x + \frac{1}{2}, \frac{5}{8}]$ | [38, 39] |
| 21 | $[\frac{1}{4} - x, \frac{5}{8}, \frac{1}{8}]$ | [41, 44] |
| 22 | $[x, \frac{1}{8}, \frac{5}{8}]$ | [42, 43] |
| 23 | $[\frac{1}{8}, \frac{5}{8}, x]$ | [45, 48] |
| 24 | $[\frac{5}{8}, \frac{1}{8}, \frac{1}{4} - x]$ | [46, 47] |

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

| No. | position | mapping |
|-----|---|----------|
| 1 | $[\frac{1}{4}, y, -y]$ | [1, 19] |
| 2 | $[0, \frac{3}{4} - y, \frac{1}{2} - y]$ | [2, 17] |
| 3 | $[\frac{1}{2}, y + \frac{1}{2}, y + \frac{1}{4}]$ | [3, 20] |
| 4 | $[\frac{3}{4}, \frac{1}{4} - y, y + \frac{3}{4}]$ | [4, 18] |
| 5 | $[-y, \frac{1}{4}, y]$ | [5, 14] |
| 6 | $[\frac{1}{2} - y, 0, \frac{3}{4} - y]$ | [6, 16] |
| 7 | $[y + \frac{1}{4}, \frac{1}{2}, y + \frac{1}{2}]$ | [7, 13] |
| 8 | $[y + \frac{3}{4}, \frac{3}{4}, \frac{1}{4} - y]$ | [8, 15] |
| 9 | $[y, -y, \frac{1}{4}]$ | [9, 24] |
| 10 | $[\frac{3}{4} - y, \frac{1}{2} - y, 0]$ | [10, 22] |
| 11 | $[y + \frac{1}{2}, y + \frac{1}{4}, \frac{1}{2}]$ | [11, 23] |
| 12 | $[\frac{1}{4} - y, y + \frac{3}{4}, \frac{3}{4}]$ | [12, 21] |
| 13 | $[\frac{3}{4}, -y, y]$ | [25, 43] |
| 14 | $[0, y + \frac{1}{4}, y + \frac{1}{2}]$ | [26, 41] |
| 15 | $[\frac{1}{2}, \frac{1}{2} - y, \frac{3}{4} - y]$ | [27, 44] |
| 16 | $[\frac{1}{4}, y + \frac{3}{4}, \frac{1}{4} - y]$ | [28, 42] |
| 17 | $[y, \frac{3}{4}, -y]$ | [29, 38] |
| 18 | $[y + \frac{1}{2}, 0, y + \frac{1}{4}]$ | [30, 40] |
| 19 | $[\frac{3}{4} - y, \frac{1}{2}, \frac{1}{2} - y]$ | [31, 37] |
| 20 | $[\frac{1}{4} - y, \frac{1}{4}, y + \frac{3}{4}]$ | [32, 39] |
| 21 | $[-y, y, \frac{3}{4}]$ | [33, 48] |
| 22 | $[y + \frac{1}{4}, y + \frac{1}{2}, 0]$ | [34, 46] |
| 23 | $[\frac{1}{2} - y, \frac{3}{4} - y, \frac{1}{2}]$ | [35, 47] |
| 24 | $[y + \frac{3}{4}, \frac{1}{4} - y, \frac{1}{4}]$ | [36, 45] |

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

| No. | position | mapping |
|-----|---|---------|
| 1 | $[x, y, z]$ | [1] |
| 2 | $[\frac{1}{4} - x, \frac{3}{4} - y, z + \frac{1}{2}]$ | [2] |
| 3 | $[\frac{3}{4} - x, y + \frac{1}{2}, \frac{1}{4} - z]$ | [3] |
| 4 | $[x + \frac{1}{2}, \frac{1}{4} - y, \frac{3}{4} - z]$ | [4] |
| 5 | $[z, x, y]$ | [5] |
| 6 | $[z + \frac{1}{2}, \frac{1}{4} - x, \frac{3}{4} - y]$ | [6] |
| 7 | $[\frac{1}{4} - z, \frac{3}{4} - x, y + \frac{1}{2}]$ | [7] |
| 8 | $[\frac{3}{4} - z, x + \frac{1}{2}, \frac{1}{4} - y]$ | [8] |
| 9 | $[y, z, x]$ | [9] |
| 10 | $[\frac{3}{4} - y, z + \frac{1}{2}, \frac{1}{4} - x]$ | [10] |
| 11 | $[y + \frac{1}{2}, \frac{1}{4} - z, \frac{3}{4} - x]$ | [11] |
| 12 | $[\frac{1}{4} - y, \frac{3}{4} - z, x + \frac{1}{2}]$ | [12] |
| 13 | $[y + \frac{3}{4}, x + \frac{1}{4}, -z]$ | [13] |
| 14 | $[\frac{1}{2} - y, \frac{1}{2} - x, \frac{1}{2} - z]$ | [14] |
| 15 | $[y + \frac{1}{4}, -x, z + \frac{3}{4}]$ | [15] |
| 16 | $[-y, x + \frac{3}{4}, z + \frac{1}{4}]$ | [16] |
| 17 | $[x + \frac{3}{4}, z + \frac{1}{4}, -y]$ | [17] |
| 18 | $[-x, z + \frac{3}{4}, y + \frac{1}{4}]$ | [18] |
| 19 | $[\frac{1}{2} - x, \frac{1}{2} - z, \frac{1}{2} - y]$ | [19] |
| 20 | $[x + \frac{1}{4}, -z, y + \frac{3}{4}]$ | [20] |
| 21 | $[z + \frac{3}{4}, y + \frac{1}{4}, -x]$ | [21] |
| 22 | $[z + \frac{1}{4}, -y, x + \frac{3}{4}]$ | [22] |
| 23 | $[-z, y + \frac{3}{4}, x + \frac{1}{4}]$ | [23] |
| 24 | $[\frac{1}{2} - z, \frac{1}{2} - y, \frac{1}{2} - x]$ | [24] |
| 25 | $[-x, -y, -z]$ | [25] |
| 26 | $[x + \frac{3}{4}, y + \frac{1}{4}, \frac{1}{2} - z]$ | [26] |
| 27 | $[x + \frac{1}{4}, \frac{1}{2} - y, z + \frac{3}{4}]$ | [27] |
| 28 | $[\frac{1}{2} - x, y + \frac{3}{4}, z + \frac{1}{4}]$ | [28] |
| 29 | $[-z, -x, -y]$ | [29] |
| 30 | $[\frac{1}{2} - z, x + \frac{3}{4}, y + \frac{1}{4}]$ | [30] |
| 31 | $[z + \frac{3}{4}, x + \frac{1}{4}, \frac{1}{2} - y]$ | [31] |
| 32 | $[z + \frac{1}{4}, \frac{1}{2} - x, y + \frac{3}{4}]$ | [32] |
| 33 | $[-y, -z, -x]$ | [33] |
| 34 | $[y + \frac{1}{4}, \frac{1}{2} - z, x + \frac{3}{4}]$ | [34] |
| 35 | $[\frac{1}{2} - y, z + \frac{3}{4}, x + \frac{1}{4}]$ | [35] |
| 36 | $[y + \frac{3}{4}, z + \frac{1}{4}, \frac{1}{2} - x]$ | [36] |
| 37 | $[\frac{1}{4} - y, \frac{3}{4} - x, z]$ | [37] |
| 38 | $[y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}]$ | [38] |
| 39 | $[\frac{3}{4} - y, x, \frac{1}{4} - z]$ | [39] |
| 40 | $[y, \frac{1}{4} - x, \frac{3}{4} - z]$ | [40] |
| 41 | $[\frac{1}{4} - x, \frac{3}{4} - z, y]$ | [41] |
| 42 | $[x, \frac{1}{4} - z, \frac{3}{4} - y]$ | [42] |
| 43 | $[x + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}]$ | [43] |
| 44 | $[\frac{3}{4} - x, z, \frac{1}{4} - y]$ | [44] |
| 45 | $[\frac{1}{4} - z, \frac{3}{4} - y, x]$ | [45] |
| 46 | $[\frac{3}{4} - z, y, \frac{1}{4} - x]$ | [46] |

continued ...

Table 8

| No. | position | mapping |
|-----|---|---------|
| 47 | $[z, \frac{1}{4} - y, \frac{3}{4} - x]$ | [47] |
| 48 | $[z + \frac{1}{2}, y + \frac{1}{2}, x + \frac{1}{2}]$ | [48] |