

MSG No. 213.64 $P4_1321'$ [Type II, cubic]

Table 1: Wyckoff site: 4a, site symmetry: .321'

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

Table 2: Wyckoff site: 4b, site symmetry: .321'

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

Table 3: Wyckoff site: 8c, site symmetry: .3.1'

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

Table 4: Wyckoff site: 12d, site symmetry: ..21'

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

continued ...

Table 4

| No. | position | mapping |
|-----|---|---------------|
| 10 | $[\frac{3}{4} - y, \frac{5}{8}, \frac{1}{2} - y]$ | [12,24,36,48] |
| 11 | $[y + \frac{1}{2}, \frac{1}{4} - y, \frac{7}{8}]$ | [15,23,39,47] |
| 12 | $[\frac{1}{2} - y, \frac{3}{4} - y, \frac{5}{8}]$ | [16,21,40,45] |

Table 5: Wyckoff site: 24e, site symmetry: 11'

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