

MSG No. 213.63 $P4_132$ [Type I, cubic]

Table 1: Wyckoff site: **4a**, site symmetry: .32

| No. | position | mapping |
|-----|---|--------------------|
| 1 | $[\frac{3}{8}, \frac{3}{8}, \frac{3}{8}]$ | [1,12,14,16,17,18] |
| 2 | $[\frac{5}{8}, \frac{7}{8}, \frac{1}{8}]$ | [2,7,9,15,19,24] |
| 3 | $[\frac{1}{8}, \frac{5}{8}, \frac{7}{8}]$ | [3,4,10,11,20,21] |
| 4 | $[\frac{7}{8}, \frac{1}{8}, \frac{5}{8}]$ | [5,6,8,13,22,23] |

Table 2: Wyckoff site: **4b**, site symmetry: .32

| No. | position | mapping |
|-----|---|--------------------|
| 1 | $[\frac{7}{8}, \frac{7}{8}, \frac{7}{8}]$ | [1,12,14,16,17,18] |
| 2 | $[\frac{1}{8}, \frac{3}{8}, \frac{5}{8}]$ | [2,7,9,15,19,24] |
| 3 | $[\frac{5}{8}, \frac{1}{8}, \frac{3}{8}]$ | [3,4,10,11,20,21] |
| 4 | $[\frac{3}{8}, \frac{5}{8}, \frac{1}{8}]$ | [5,6,8,13,22,23] |

Table 3: Wyckoff site: **8c**, site symmetry: .3.

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

Table 4: Wyckoff site: **12d**, site symmetry: ..2

| No. | position | mapping |
|-----|---|---------|
| 1 | $[\frac{1}{8}, y, y + \frac{1}{4}]$ | [1,13] |
| 2 | $[\frac{3}{8}, -y, y + \frac{3}{4}]$ | [2,10] |
| 3 | $[\frac{7}{8}, y + \frac{1}{2}, \frac{1}{4} - y]$ | [3,9] |
| 4 | $[y, y + \frac{1}{4}, \frac{1}{8}]$ | [4,18] |
| 5 | $[-y, y + \frac{3}{4}, \frac{3}{8}]$ | [5,19] |
| 6 | $[\frac{1}{4} - y, \frac{7}{8}, y + \frac{1}{2}]$ | [6,20] |
| 7 | $[y + \frac{1}{4}, \frac{1}{8}, y]$ | [7,17] |
| 8 | $[\frac{5}{8}, \frac{1}{2} - y, \frac{3}{4} - y]$ | [8,14] |
| 9 | $[y + \frac{3}{4}, \frac{3}{8}, -y]$ | [11,22] |

continued ...

Table 4

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

Table 5: Wyckoff site: 24e, site symmetry: 1

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