

MSG No. 61.438 $P_a bca$ [Type IV, orthorhombic]

Table 1: Wyckoff site: **8a**, site symmetry: $-1'$

| No. | position | mapping |
|-----|---|---------|
| 1 | $[\frac{3}{4}, 0, 0]$ | [1,13] |
| 2 | $[\frac{1}{4}, \frac{1}{2}, 0]$ | [2,14] |
| 3 | $[\frac{1}{4}, \frac{1}{2}, \frac{1}{2}]$ | [3,15] |
| 4 | $[\frac{3}{4}, 0, \frac{1}{2}]$ | [4,16] |
| 5 | $[\frac{1}{4}, 0, 0]$ | [5,9] |
| 6 | $[\frac{3}{4}, \frac{1}{2}, 0]$ | [6,10] |
| 7 | $[\frac{3}{4}, \frac{1}{2}, \frac{1}{2}]$ | [7,11] |
| 8 | $[\frac{1}{4}, 0, \frac{1}{2}]$ | [8,12] |

Table 2: Wyckoff site: **8b**, site symmetry: -1

| No. | position | mapping |
|-----|---|---------|
| 1 | $[0, 0, 0]$ | [1,5] |
| 2 | $[\frac{1}{2}, \frac{1}{2}, 0]$ | [2,6] |
| 3 | $[0, \frac{1}{2}, \frac{1}{2}]$ | [3,7] |
| 4 | $[\frac{1}{2}, 0, \frac{1}{2}]$ | [4,8] |
| 5 | $[\frac{1}{2}, 0, 0]$ | [9,13] |
| 6 | $[0, \frac{1}{2}, 0]$ | [10,14] |
| 7 | $[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$ | [11,15] |
| 8 | $[0, 0, \frac{1}{2}]$ | [12,16] |

Table 3: Wyckoff site: **8c**, site symmetry: $2'..$

| No. | position | mapping |
|-----|---|---------|
| 1 | $[x, \frac{1}{4}, 0]$ | [1,10] |
| 2 | $[x + \frac{1}{2}, \frac{1}{4}, 0]$ | [2,9] |
| 3 | $[-x, \frac{3}{4}, \frac{1}{2}]$ | [3,12] |
| 4 | $[\frac{1}{2} - x, \frac{3}{4}, \frac{1}{2}]$ | [4,11] |
| 5 | $[-x, \frac{3}{4}, 0]$ | [5,14] |
| 6 | $[\frac{1}{2} - x, \frac{3}{4}, 0]$ | [6,13] |
| 7 | $[x, \frac{1}{4}, \frac{1}{2}]$ | [7,16] |
| 8 | $[x + \frac{1}{2}, \frac{1}{4}, \frac{1}{2}]$ | [8,15] |

Table 4: Wyckoff site: **8d**, site symmetry: $\bar{3}m'$

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

Table 5: Wyckoff site: **16e**, site symmetry: $\bar{1}$

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