

MSG No. 102.187  $P4_2nm$  [ Type I, tetragonal ]

Table 1: Wyckoff site: 2a, site symmetry: 2..mm

| No. | position                                    | mapping      |
|-----|---|--------------|
| 1   | [0, 0, z]                                   | [1, 4, 7, 8] |
| 2   | [\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}] | [2, 3, 5, 6] |

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

| No. | position                          | mapping |
|-----|-----------------------------------|---------|
| 1   | [0, \frac{1}{2}, z]               | [1, 4]  |
| 2   | [0, \frac{1}{2}, z + \frac{1}{2}] | [2, 3]  |
| 3   | [\frac{1}{2}, 0, z + \frac{1}{2}] | [5, 6]  |
| 4   | [\frac{1}{2}, 0, z]               | [7, 8]  |

Table 3: Wyckoff site: 4c, site symmetry: ...m

| No. | position  | mapping |
|-----|---|---------|
| 1   | [x, x, z]   | [1, 8]  |
| 2   | [\frac{1}{2} - x, x + \frac{1}{2}, z + \frac{1}{2}] | [2, 5]  |
| 3   | [x + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}] | [3, 6]  |
| 4   | [-x, -x, z]   | [4, 7]  |

Table 4: Wyckoff site: 8d, site symmetry: 1

| No. | position  | mapping |
|-----|---|---------|
| 1   | [x, y, z]   | [1]     |
| 2   | [\frac{1}{2} - y, x + \frac{1}{2}, z + \frac{1}{2}] | [2]     |
| 3   | [y + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}] | [3]     |
| 4   | [-x, -y, z]   | [4]     |
| 5   | [\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}] | [5]     |
| 6   | [x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}] | [6]     |
| 7   | [-y, -x, z]   | [7]     |
| 8   | [y, x, z]   | [8]     |