

MSG No. 106.220 $P4_2bc1'$ [Type II, tetragonal]

Table 1: Wyckoff site: 4a, site symmetry: 2..1'

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

Table 2: Wyckoff site: 4b, site symmetry: 2..1'

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

Table 3: Wyckoff site: 8c, site symmetry: 11'

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