

MSG No. 59.406 *Pmmn1'* [Type II, orthorhombic]

Table 1: Wyckoff site: 2a, site symmetry: **mm21'**

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

Table 2: Wyckoff site: 2b, site symmetry: **mm21'**

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

Table 3: Wyckoff site: 4c, site symmetry: **-11'**

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

Table 4: Wyckoff site: 4d, site symmetry: **-11'**

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

Table 5: Wyckoff site: 4e, site symmetry: **m..1'**

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

Table 6: Wyckoff site: 4f, site symmetry: .m.1'

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

Table 7: Wyckoff site: 8g, site symmetry: 11'

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