

MSG No. 20.32 $C222_11'$ [Type II, orthorhombic]

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

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

Table 2: Wyckoff site: 4b, site symmetry: .2.1'

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

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

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