

MSG No. 26.75 P_Bmc2_1 [Type IV, orthorhombic]

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

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

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

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

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

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

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

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