

MSG No. 36.172 $Cmc2_1$ [Type I, orthorhombic]

Table 1: Wyckoff site: **4a**, site symmetry: $m..$

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

Table 2: Wyckoff site: **8b**, 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 | $[x + \frac{1}{2}, y + \frac{1}{2}, z]$ | $[5]$ |
| 6 | $[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$ | $[6]$ |
| 7 | $[\frac{1}{2} - x, y + \frac{1}{2}, z]$ | $[7]$ |
| 8 | $[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$ | $[8]$ |