

MSG No. 26.66  $Pmc2_1$  [ Type I, orthorhombic ]

Table 1: Wyckoff site: 2a, site symmetry:  $m . .$

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

Table 2: Wyckoff site: 2b, site symmetry:  $m . .$

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

Table 3: Wyckoff site: 4c, 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   | $[x, -y, z + \frac{1}{2}]$  | $[4]$   |