

MSG No. 30.114 $Pnc'2'$ [Type III, orthorhombic]

Table 1: Wyckoff site: 2a, site symmetry: $\dots 2'$

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

Table 2: Wyckoff site: 2b, site symmetry: $\dots 2'$

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

Table 3: Wyckoff site: 4c, site symmetry: 1

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