

SG No. 34 C_{2v}^{10} $Pnn2$ [orthorhombic]

* plus set: $+ [0, 0, 0]$

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

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

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

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

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

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