

SG No. 36 C_{2v}^{12} $Cmc2_1$ [orthorhombic]

* plus set: $+ [0, 0, 0], + [\frac{1}{2}, \frac{1}{2}, 0]$

* Wyckoff site: **4a**, site symmetry: **m** . .

Table 1: Wyckoff bond: **4a@4a**

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

Table 2: Wyckoff bond: **4b@4a**

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

Table 3: Wyckoff bond: **8c@4a**

| No. | vector | center | mapping |
|-----|---------------|----------------------------|---------|
| 1 | $[X, Y, Z]$ | $[0, y, z]$ | $[1]$ |
| 2 | $[-X, -Y, Z]$ | $[0, -y, z + \frac{1}{2}]$ | $[2]$ |
| 3 | $[X, -Y, Z]$ | $[0, -y, z + \frac{1}{2}]$ | $[3]$ |
| 4 | $[-X, Y, Z]$ | $[0, y, z]$ | $[4]$ |

* Wyckoff site: **8b**, site symmetry: **1**

Table 4: Wyckoff bond: **8a@8b**

| No. | vector | center | mapping |
|-----|---------------|-----------------------------|---------|
| 1 | $[X, Y, Z]$ | $[x, y, z]$ | $[1]$ |
| 2 | $[-X, -Y, Z]$ | $[-x, -y, z + \frac{1}{2}]$ | $[2]$ |
| 3 | $[X, -Y, Z]$ | $[x, -y, z + \frac{1}{2}]$ | $[3]$ |
| 4 | $[-X, Y, Z]$ | $[-x, y, z]$ | $[4]$ |