

SG No. 37 C_{2v}^{13} $Ccc2$ [orthorhombic]

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

* Wyckoff site: **4a**, site symmetry: $\dots 2$

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

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

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

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

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

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

* Wyckoff site: **4b**, site symmetry: $\dots 2$

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

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

Table 5: Wyckoff bond: **4b@4b**

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

Table 6: Wyckoff bond: **8c@4b**

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

* Wyckoff site: **4c**, site symmetry: $\dots 2$

Table 7: Wyckoff bond: **4a@4c**

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

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

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

Table 9: Wyckoff bond: **8c@4c**

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

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

Table 10: Wyckoff bond: **8a@8d**

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