

PG No. 3  $C_2$  2 (b-axis setting) [ monoclinic ]

\* Wyckoff site: 1a, site symmetry: 2

Table 1: Wyckoff bond: 1a@1a

| No. | vector      | center      | mapping   |
|-----|-------------|-------------|-----------|
| 1   | $[X, 0, Z]$ | $[0, y, 0]$ | $[1, -2]$ |

Table 2: Wyckoff bond: 1b@1a

| No. | vector      | center      | mapping  |
|-----|-------------|-------------|----------|
| 1   | $[0, Y, 0]$ | $[0, y, 0]$ | $[1, 2]$ |

Table 3: Wyckoff bond: 2c@1a

| No. | vector        | center      | mapping |
|-----|---------------|-------------|---------|
| 1   | $[X, Y, Z]$   | $[0, y, 0]$ | $[1]$   |
| 2   | $[-X, Y, -Z]$ | $[0, y, 0]$ | $[2]$   |

\* Wyckoff site: 2b, site symmetry: 1

Table 4: Wyckoff bond: 2a@2b

| No. | vector        | center        | mapping |
|-----|---------------|---------------|---------|
| 1   | $[X, Y, Z]$   | $[x, y, z]$   | $[1]$   |
| 2   | $[-X, Y, -Z]$ | $[-x, y, -z]$ | $[2]$   |