

Table 1: Wyckoff site: 2a, site symmetry: 4..

| No. | position                  | mapping        |
|-----|---------------------------|----------------|
| 1   | $[0, 0, z]$               | $[1, 2, 3, 4]$ |
| 2   | $[0, 0, z + \frac{1}{2}]$ | $[5, 6, 7, 8]$ |

Table 2: Wyckoff site: 2b, site symmetry: 4..

| No. | position                                      | mapping        |
|-----|---|----------------|
| 1   | $[\frac{1}{2}, \frac{1}{2}, z]$               | $[1, 2, 3, 4]$ |
| 2   | $[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$ | $[5, 6, 7, 8]$ |

Table 3: Wyckoff site: 4c, site symmetry: 2..

| No. | position                            | mapping  |
|-----|-------------------------------------|----------|
| 1   | $[0, \frac{1}{2}, z]$               | $[1, 4]$ |
| 2   | $[\frac{1}{2}, 0, z]$               | $[2, 3]$ |
| 3   | $[0, \frac{1}{2}, z + \frac{1}{2}]$ | $[5, 6]$ |
| 4   | $[\frac{1}{2}, 0, z + \frac{1}{2}]$ | $[7, 8]$ |

Table 4: Wyckoff site: 8d, site symmetry: 1

| No. | position                    | mapping |
|-----|-----------------------------|---------|
| 1   | $[x, y, z]$                 | $[1]$   |
| 2   | $[-y, x, z]$                | $[2]$   |
| 3   | $[y, -x, z]$                | $[3]$   |
| 4   | $[-x, -y, z]$               | $[4]$   |
| 5   | $[-x, y, z + \frac{1}{2}]$  | $[5]$   |
| 6   | $[x, -y, z + \frac{1}{2}]$  | $[6]$   |
| 7   | $[-y, -x, z + \frac{1}{2}]$ | $[7]$   |
| 8   | $[y, x, z + \frac{1}{2}]$   | $[8]$   |