

Table 1: Wyckoff site: **4a**, site symmetry:  $\cdot\cdot 2$

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

Table 2: Wyckoff site: **4b**, site symmetry:  $\mathbf{m}\cdot\cdot$

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

Table 3: Wyckoff site: **8c**, site symmetry:  $\mathbf{1}$

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