

Table 1: Wyckoff site: **2a**, site symmetry:  $2.m'm'$

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

Table 2: Wyckoff site: **2b**, site symmetry:  $2.m'm'$

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

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

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

Table 4: Wyckoff site: **4d**, site symmetry:  $..m'$

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

Table 5: Wyckoff site: **8e**, site symmetry:  $1$

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

*continued ...*

Table 5

| No. | position      | mapping |
|-----|---------------|---------|
| 7   | $[-y, -x, z]$ | [7]     |
| 8   | $[y, x, z]$   | [8]     |