

Table 1: Wyckoff site: **4a**, site symmetry:  $-1'$ 

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

Table 2: Wyckoff site: **4b**, site symmetry:  $-1'$ 

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

Table 3: Wyckoff site: **4c**, site symmetry:  $\dots 2'$ 

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

Table 4: Wyckoff site: **4d**, site symmetry:  $2..$ 

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

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

| No. | position                                | mapping |
|-----|---|---------|
| 1   | $[x, y, z]$                             | $[1]$   |
| 2   | $[x, \frac{1}{2} - y, \frac{1}{2} - z]$ | $[2]$   |

*continued ...*

Table 5

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