

SG No. 66 D_{2h}^{20} $Cccm$ [orthorhombic]

* plus set: $+ [0, 0, 0]$, $+ [\frac{1}{2}, \frac{1}{2}, 0]$

Table 1: Wyckoff site: 4a, site symmetry: 222

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

Table 2: Wyckoff site: 4b, site symmetry: 222

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

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

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

Table 4: Wyckoff site: 4d, site symmetry: . .2/m

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

Table 5: Wyckoff site: 4e, site symmetry: . .2/m

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

Table 6: Wyckoff site: 4f, site symmetry: . . 2/m

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

Table 7: Wyckoff site: 8g, site symmetry: 2..

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

Table 8: Wyckoff site: 8h, site symmetry: . 2.

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

Table 9: Wyckoff site: 8i, site symmetry: .. 2

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

Table 10: Wyckoff site: 8j, site symmetry: .. 2

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

Table 11: Wyckoff site: 8k, site symmetry: . . 2

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

Table 12: Wyckoff site: 8l, site symmetry: . . m

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

Table 13: Wyckoff site: 16m, site symmetry: 1

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