

MSG No. 14.84 P_C2_1/c [Type IV, monoclinic]

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

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

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

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

Table 3: Wyckoff site: **4c**, site symmetry: -1

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

Table 4: Wyckoff site: **4d**, site symmetry: -1

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

Table 5: Wyckoff site: **4e**, site symmetry: $2'$

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

continued ...

Table 5

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

Table 6: Wyckoff site: 8f, site symmetry: 1

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