

MSG No. 13.69 $P2'/c'$ [Type III, monoclinic]

Table 1: Wyckoff site: 2a, site symmetry: -1

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

Table 2: Wyckoff site: 2b, site symmetry: -1

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

Table 3: Wyckoff site: 2c, site symmetry: -1

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

Table 4: Wyckoff site: 2d, site symmetry: -1

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

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

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

Table 6: Wyckoff site: 2f, site symmetry: $2'$

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

Table 7: Wyckoff site: $4g$, 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 | $[x, -y, z + \frac{1}{2}]$ | [4] |