

MSG No. 13.65  $P2/c$  [ Type I, monoclinic ]

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

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

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

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

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

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

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

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

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

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

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

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

Table 7: Wyckoff site:  $4g$ , site symmetry:  $1$ 

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