

MSG No. 14.78  $P2_1/c'$  [ Type III, monoclinic ]

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

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

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

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

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

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

Table 5: Wyckoff site: 4e, 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]     |