

SG No. 21  $D_2^6$  C222 [ orthorhombic ]

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

Table 1: Wyckoff site: 2a, site symmetry: 222

| No. | position    | mapping        |
|-----|-------------|----------------|
| 1   | $[0, 0, 0]$ | $[1, 2, 3, 4]$ |

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

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

Table 3: Wyckoff site: 2c, site symmetry: 222

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

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

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

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

| No. | position     | mapping  |
|-----|--------------|----------|
| 1   | $[x, 0, 0]$  | $[1, 4]$ |
| 2   | $[-x, 0, 0]$ | $[2, 3]$ |

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

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

Table 7: Wyckoff site: 4g, site symmetry: .2.

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

Table 8: Wyckoff site: 4h, site symmetry: .2.

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

Table 9: Wyckoff site: 4i, site symmetry: ..2

| No. | position      | mapping |
|-----|---------------|---------|
| 1   | [0, 0, $z$ ]  | [1,2]   |
| 2   | [0, 0, $-z$ ] | [3,4]   |

Table 10: Wyckoff site: 4j, site symmetry: ..2

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

Table 11: Wyckoff site: 4k, site symmetry: ..2

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

Table 12: Wyckoff site: 8l, site symmetry: 1

| No. | position              | mapping |
|-----|-----------------------|---------|
| 1   | [ $x$ , $y$ , $z$ ]   | [1]     |
| 2   | [ $-x$ , $-y$ , $z$ ] | [2]     |
| 3   | [ $-x$ , $y$ , $-z$ ] | [3]     |
| 4   | [ $x$ , $-y$ , $-z$ ] | [4]     |