

SG No. 74  $D_{2h}^{28}$  *Imma* [ orthorhombic ]

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

\* Wyckoff site: 4a, site symmetry: 2/m..

Table 1: Wyckoff bond: 4a@4a

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

Table 2: Wyckoff bond: 4b@4a

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

Table 3: Wyckoff bond: 8c@4a

| No. | vector        | center                | mapping   |
|-----|---------------|-----------------------|-----------|
| 1   | $[X, Y, Z]$   | $[0, 0, 0]$           | $[1, -5]$ |
| 2   | $[-X, -Y, Z]$ | $[0, \frac{1}{2}, 0]$ | $[2, -6]$ |
| 3   | $[-X, Y, -Z]$ | $[0, \frac{1}{2}, 0]$ | $[3, -7]$ |
| 4   | $[X, -Y, -Z]$ | $[0, 0, 0]$           | $[4, -8]$ |

\* Wyckoff site: 4b, site symmetry: 2/m..

Table 4: Wyckoff bond: 4a@4b

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

Table 5: Wyckoff bond: 4b@4b

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

Table 6: Wyckoff bond: 8c@4b

| No. | vector        | center                          | mapping   |
|-----|---------------|---------------------------------|-----------|
| 1   | $[X, Y, Z]$   | $[0, 0, \frac{1}{2}]$           | $[1, -5]$ |
| 2   | $[-X, -Y, Z]$ | $[0, \frac{1}{2}, \frac{1}{2}]$ | $[2, -6]$ |
| 3   | $[-X, Y, -Z]$ | $[0, \frac{1}{2}, \frac{1}{2}]$ | $[3, -7]$ |
| 4   | $[X, -Y, -Z]$ | $[0, 0, \frac{1}{2}]$           | $[4, -8]$ |

\* Wyckoff site: 4c, site symmetry: .2/m.

Table 7: Wyckoff bond: 4a@4c

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

Table 8: Wyckoff bond: 4b@4c

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

Table 9: Wyckoff bond: 8c@4c

| No. | vector        | center                                    | mapping   |
|-----|---------------|---|-----------|
| 1   | $[X, Y, Z]$   | $[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$ | $[1, -5]$ |
| 2   | $[-X, -Y, Z]$ | $[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$ | $[2, -6]$ |
| 3   | $[-X, Y, -Z]$ | $[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$ | $[3, -7]$ |
| 4   | $[X, -Y, -Z]$ | $[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$ | $[4, -8]$ |

\* Wyckoff site: 4d, site symmetry: .2/m.

Table 10: Wyckoff bond: 4a@4d

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

Table 11: Wyckoff bond: 4b@4d

| No. | vector     | center   | mapping     |
|-----|------------|--|-------------|
| 1   | [0, Y, 0]  | $\left[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}\right]$ | [1,3,-5,-7] |
| 2   | [0, -Y, 0] | $\left[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}\right]$ | [2,4,-6,-8] |

Table 12: Wyckoff bond: 8c@4d

| No. | vector      | center   | mapping |
|-----|-------------|--|---------|
| 1   | [X, Y, Z]   | $\left[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}\right]$ | [1,-5]  |
| 2   | [-X, -Y, Z] | $\left[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}\right]$ | [2,-6]  |
| 3   | [-X, Y, -Z] | $\left[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}\right]$ | [3,-7]  |
| 4   | [X, -Y, -Z] | $\left[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}\right]$ | [4,-8]  |

\* Wyckoff site: 4e, site symmetry: mm2

Table 13: Wyckoff bond: 4a@4e

| No. | vector     | center                            | mapping   |
|-----|------------|-----------------------------------|-----------|
| 1   | [0, 0, Z]  | $\left[0, \frac{1}{4}, z\right]$  | [1,2,7,8] |
| 2   | [0, 0, -Z] | $\left[0, \frac{3}{4}, -z\right]$ | [3,4,5,6] |

Table 14: Wyckoff bond: 4b@4e

| No. | vector    | center                            | mapping     |
|-----|-----------|-----------------------------------|-------------|
| 1   | [0, Y, 0] | $\left[0, \frac{1}{4}, z\right]$  | [1,-2,-7,8] |
| 2   | [0, Y, 0] | $\left[0, \frac{3}{4}, -z\right]$ | [3,-4,-5,6] |

Table 15: Wyckoff bond: 4c@4e

| No. | vector     | center                            | mapping     |
|-----|------------|-----------------------------------|-------------|
| 1   | [X, 0, 0]  | $\left[0, \frac{1}{4}, z\right]$  | [1,-2,7,-8] |
| 2   | [-X, 0, 0] | $\left[0, \frac{3}{4}, -z\right]$ | [3,-4,5,-6] |

Table 16: Wyckoff bond: 8d@4e

| No. | vector        | center                 | mapping |
|-----|---------------|------------------------|---------|
| 1   | $[X, Y, 0]$   | $[0, \frac{1}{4}, z]$  | [1,-2]  |
| 2   | $[-X, Y, 0]$  | $[0, \frac{3}{4}, -z]$ | [3,-4]  |
| 3   | $[-X, -Y, 0]$ | $[0, \frac{3}{4}, -z]$ | [5,-6]  |
| 4   | $[X, -Y, 0]$  | $[0, \frac{1}{4}, z]$  | [7,-8]  |

Table 17: Wyckoff bond: 8e@4e

| No. | vector        | center                 | mapping |
|-----|---------------|------------------------|---------|
| 1   | $[X, 0, Z]$   | $[0, \frac{1}{4}, z]$  | [1,7]   |
| 2   | $[-X, 0, Z]$  | $[0, \frac{1}{4}, z]$  | [2,8]   |
| 3   | $[-X, 0, -Z]$ | $[0, \frac{3}{4}, -z]$ | [3,5]   |
| 4   | $[X, 0, -Z]$  | $[0, \frac{3}{4}, -z]$ | [4,6]   |

Table 18: Wyckoff bond: 8f@4e

| No. | vector        | center                 | mapping |
|-----|---------------|------------------------|---------|
| 1   | $[0, Y, Z]$   | $[0, \frac{1}{4}, z]$  | [1,8]   |
| 2   | $[0, -Y, Z]$  | $[0, \frac{1}{4}, z]$  | [2,7]   |
| 3   | $[0, Y, -Z]$  | $[0, \frac{3}{4}, -z]$ | [3,6]   |
| 4   | $[0, -Y, -Z]$ | $[0, \frac{3}{4}, -z]$ | [4,5]   |

Table 19: Wyckoff bond: 16g@4e

| No. | vector         | center                 | mapping |
|-----|----------------|------------------------|---------|
| 1   | $[X, Y, Z]$    | $[0, \frac{1}{4}, z]$  | [1]     |
| 2   | $[-X, -Y, Z]$  | $[0, \frac{1}{4}, z]$  | [2]     |
| 3   | $[-X, Y, -Z]$  | $[0, \frac{3}{4}, -z]$ | [3]     |
| 4   | $[X, -Y, -Z]$  | $[0, \frac{3}{4}, -z]$ | [4]     |
| 5   | $[-X, -Y, -Z]$ | $[0, \frac{3}{4}, -z]$ | [5]     |
| 6   | $[X, Y, -Z]$   | $[0, \frac{3}{4}, -z]$ | [6]     |
| 7   | $[X, -Y, Z]$   | $[0, \frac{1}{4}, z]$  | [7]     |
| 8   | $[-X, Y, Z]$   | $[0, \frac{1}{4}, z]$  | [8]     |

\* Wyckoff site: 8f, site symmetry: 2..

Table 20: Wyckoff bond: 8a@8f

| No. | vector      | center                  | mapping |
|-----|-------------|-------------------------|---------|
| 1   | [0, Y, Z]   | [x, 0, 0]               | [1, -4] |
| 2   | [0, -Y, Z]  | [-x, $\frac{1}{2}$ , 0] | [2, -3] |
| 3   | [0, -Y, -Z] | [-x, 0, 0]              | [5, -8] |
| 4   | [0, Y, -Z]  | [x, $\frac{1}{2}$ , 0]  | [6, -7] |

Table 21: Wyckoff bond: 8b@8f

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

Table 22: Wyckoff bond: 16c@8f

| No. | vector       | center                  | mapping |
|-----|--------------|-------------------------|---------|
| 1   | [X, Y, Z]    | [x, 0, 0]               | [1]     |
| 2   | [-X, -Y, Z]  | [-x, $\frac{1}{2}$ , 0] | [2]     |
| 3   | [-X, Y, -Z]  | [-x, $\frac{1}{2}$ , 0] | [3]     |
| 4   | [X, -Y, -Z]  | [x, 0, 0]               | [4]     |
| 5   | [-X, -Y, -Z] | [-x, 0, 0]              | [5]     |
| 6   | [X, Y, -Z]   | [x, $\frac{1}{2}$ , 0]  | [6]     |
| 7   | [X, -Y, Z]   | [x, $\frac{1}{2}$ , 0]  | [7]     |
| 8   | [-X, Y, Z]   | [-x, 0, 0]              | [8]     |

\* Wyckoff site: 8g, site symmetry: .2.

Table 23: Wyckoff bond: 8a@8g

| No. | vector      | center   | mapping |
|-----|-------------|--|---------|
| 1   | [X, 0, Z]   | [\mathbf{\frac{1}{4}}, y, \mathbf{\frac{1}{4}}]                        | [1, -3] |
| 2   | [-X, 0, Z]  | [\mathbf{\frac{3}{4}}, \mathbf{\frac{1}{2}} - y, \mathbf{\frac{1}{4}}] | [2, -4] |
| 3   | [-X, 0, -Z] | [\mathbf{\frac{3}{4}}, -y, \mathbf{\frac{3}{4}}]                       | [5, -7] |
| 4   | [X, 0, -Z]  | [\mathbf{\frac{1}{4}}, y + \mathbf{\frac{1}{2}}, \mathbf{\frac{3}{4}}] | [6, -8] |

Table 24: Wyckoff bond: 8b@8g

| No. | vector     | center  | mapping |
|-----|------------|---|---------|
| 1   | [0, Y, 0]  | $[\frac{1}{4}, y, \frac{1}{4}]$               | [1,3]   |
| 2   | [0, -Y, 0] | $[\frac{3}{4}, \frac{1}{2} - y, \frac{1}{4}]$ | [2,4]   |
| 3   | [0, -Y, 0] | $[\frac{3}{4}, -y, \frac{3}{4}]$              | [5,7]   |
| 4   | [0, Y, 0]  | $[\frac{1}{4}, y + \frac{1}{2}, \frac{3}{4}]$ | [6,8]   |

Table 25: Wyckoff bond: 16c@8g

| No. | vector       | center  | mapping |
|-----|--------------|---|---------|
| 1   | [X, Y, Z]    | $[\frac{1}{4}, y, \frac{1}{4}]$               | [1]     |
| 2   | [-X, -Y, Z]  | $[\frac{3}{4}, \frac{1}{2} - y, \frac{1}{4}]$ | [2]     |
| 3   | [-X, Y, -Z]  | $[\frac{1}{4}, y, \frac{1}{4}]$               | [3]     |
| 4   | [X, -Y, -Z]  | $[\frac{3}{4}, \frac{1}{2} - y, \frac{1}{4}]$ | [4]     |
| 5   | [-X, -Y, -Z] | $[\frac{3}{4}, -y, \frac{3}{4}]$              | [5]     |
| 6   | [X, Y, -Z]   | $[\frac{1}{4}, y + \frac{1}{2}, \frac{3}{4}]$ | [6]     |
| 7   | [X, -Y, Z]   | $[\frac{3}{4}, -y, \frac{3}{4}]$              | [7]     |
| 8   | [-X, Y, Z]   | $[\frac{1}{4}, y + \frac{1}{2}, \frac{3}{4}]$ | [8]     |

\* Wyckoff site: 8h, site symmetry: m..

Table 26: Wyckoff bond: 8a@8h

| No. | vector      | center                     | mapping |
|-----|-------------|----------------------------|---------|
| 1   | [0, Y, Z]   | [0, y, z]                  | [1,8]   |
| 2   | [0, -Y, Z]  | $[0, \frac{1}{2} - y, z]$  | [2,7]   |
| 3   | [0, Y, -Z]  | $[0, y + \frac{1}{2}, -z]$ | [3,6]   |
| 4   | [0, -Y, -Z] | $[0, -y, -z]$              | [4,5]   |

Table 27: Wyckoff bond: 8b@8h

| No. | vector     | center                     | mapping |
|-----|------------|----------------------------|---------|
| 1   | [X, 0, 0]  | [0, y, z]                  | [1,-8]  |
| 2   | [-X, 0, 0] | $[0, \frac{1}{2} - y, z]$  | [2,-7]  |
| 3   | [-X, 0, 0] | $[0, y + \frac{1}{2}, -z]$ | [3,-6]  |
| 4   | [X, 0, 0]  | $[0, -y, -z]$              | [4,-5]  |

Table 28: Wyckoff bond: 16c@8h

| No. | vector         | center                     | mapping |
|-----|----------------|----------------------------|---------|
| 1   | $[X, Y, Z]$    | $[0, y, z]$                | [1]     |
| 2   | $[-X, -Y, Z]$  | $[0, \frac{1}{2} - y, z]$  | [2]     |
| 3   | $[-X, Y, -Z]$  | $[0, y + \frac{1}{2}, -z]$ | [3]     |
| 4   | $[X, -Y, -Z]$  | $[0, -y, -z]$              | [4]     |
| 5   | $[-X, -Y, -Z]$ | $[0, -y, -z]$              | [5]     |
| 6   | $[X, Y, -Z]$   | $[0, y + \frac{1}{2}, -z]$ | [6]     |
| 7   | $[X, -Y, Z]$   | $[0, \frac{1}{2} - y, z]$  | [7]     |
| 8   | $[-X, Y, Z]$   | $[0, y, z]$                | [8]     |

\* Wyckoff site: 8i, site symmetry: .m.

Table 29: Wyckoff bond: 8a@8i

| No. | vector        | center                  | mapping |
|-----|---------------|-------------------------|---------|
| 1   | $[X, 0, Z]$   | $[x, \frac{1}{4}, z]$   | [1,7]   |
| 2   | $[-X, 0, Z]$  | $[-x, \frac{1}{4}, z]$  | [2,8]   |
| 3   | $[-X, 0, -Z]$ | $[-x, \frac{3}{4}, -z]$ | [3,5]   |
| 4   | $[X, 0, -Z]$  | $[x, \frac{3}{4}, -z]$  | [4,6]   |

Table 30: Wyckoff bond: 8b@8i

| No. | vector       | center                  | mapping |
|-----|--------------|-------------------------|---------|
| 1   | $[0, Y, 0]$  | $[x, \frac{1}{4}, z]$   | [1,-7]  |
| 2   | $[0, -Y, 0]$ | $[-x, \frac{1}{4}, z]$  | [2,-8]  |
| 3   | $[0, Y, 0]$  | $[-x, \frac{3}{4}, -z]$ | [3,-5]  |
| 4   | $[0, -Y, 0]$ | $[x, \frac{3}{4}, -z]$  | [4,-6]  |

Table 31: Wyckoff bond: 16c@8i

| No. | vector         | center                  | mapping |
|-----|----------------|-------------------------|---------|
| 1   | $[X, Y, Z]$    | $[x, \frac{1}{4}, z]$   | [1]     |
| 2   | $[-X, -Y, Z]$  | $[-x, \frac{1}{4}, z]$  | [2]     |
| 3   | $[-X, Y, -Z]$  | $[-x, \frac{3}{4}, -z]$ | [3]     |
| 4   | $[X, -Y, -Z]$  | $[x, \frac{3}{4}, -z]$  | [4]     |
| 5   | $[-X, -Y, -Z]$ | $[-x, \frac{3}{4}, -z]$ | [5]     |
| 6   | $[X, Y, -Z]$   | $[x, \frac{3}{4}, -z]$  | [6]     |
| 7   | $[X, -Y, Z]$   | $[x, \frac{1}{4}, z]$   | [7]     |
| 8   | $[-X, Y, Z]$   | $[-x, \frac{1}{4}, z]$  | [8]     |

\* Wyckoff site: 16j, site symmetry: 1

Table 32: Wyckoff bond: 16a@16j

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