

SG No. 142 D_{4h}^{20} $I4_1/acd$ [tetragonal]

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

* Wyckoff site: **8a**, site symmetry: $-4..$

Table 1: Wyckoff bond: **8a@8a**

| No. | vector | center | mapping |
|-----|--------------|---|--------------------|
| 1 | $[0, 0, Z]$ | $[0, \frac{1}{4}, \frac{3}{8}]$ | $[1, 2, -11, -12]$ |
| 2 | $[0, 0, Z]$ | $[0, \frac{3}{4}, \frac{5}{8}]$ | $[3, 4, -9, -10]$ |
| 3 | $[0, 0, -Z]$ | $[\frac{1}{2}, \frac{1}{4}, \frac{5}{8}]$ | $[5, 6, -15, -16]$ |
| 4 | $[0, 0, -Z]$ | $[\frac{1}{2}, \frac{3}{4}, \frac{3}{8}]$ | $[7, 8, -13, -14]$ |

Table 2: Wyckoff bond: **16b@8a**

| No. | vector | center | mapping |
|-----|---------------|---|-------------|
| 1 | $[X, Y, 0]$ | $[0, \frac{1}{4}, \frac{3}{8}]$ | $[1, -2]$ |
| 2 | $[-Y, X, 0]$ | $[0, \frac{3}{4}, \frac{5}{8}]$ | $[3, -4]$ |
| 3 | $[-X, Y, 0]$ | $[\frac{1}{2}, \frac{1}{4}, \frac{5}{8}]$ | $[5, -6]$ |
| 4 | $[Y, X, 0]$ | $[\frac{1}{2}, \frac{3}{4}, \frac{3}{8}]$ | $[7, -8]$ |
| 5 | $[-X, -Y, 0]$ | $[0, \frac{3}{4}, \frac{5}{8}]$ | $[9, -10]$ |
| 6 | $[Y, -X, 0]$ | $[0, \frac{1}{4}, \frac{3}{8}]$ | $[11, -12]$ |
| 7 | $[X, -Y, 0]$ | $[\frac{1}{2}, \frac{3}{4}, \frac{3}{8}]$ | $[13, -14]$ |
| 8 | $[-Y, -X, 0]$ | $[\frac{1}{2}, \frac{1}{4}, \frac{5}{8}]$ | $[15, -16]$ |

Table 3: Wyckoff bond: **32c@8a**

| No. | vector | center | mapping |
|-----|----------------|---|---------|
| 1 | $[X, Y, Z]$ | $[0, \frac{1}{4}, \frac{3}{8}]$ | $[1]$ |
| 2 | $[-X, -Y, Z]$ | $[0, \frac{1}{4}, \frac{3}{8}]$ | $[2]$ |
| 3 | $[-Y, X, Z]$ | $[0, \frac{3}{4}, \frac{5}{8}]$ | $[3]$ |
| 4 | $[Y, -X, Z]$ | $[0, \frac{3}{4}, \frac{5}{8}]$ | $[4]$ |
| 5 | $[-X, Y, -Z]$ | $[\frac{1}{2}, \frac{1}{4}, \frac{5}{8}]$ | $[5]$ |
| 6 | $[X, -Y, -Z]$ | $[\frac{1}{2}, \frac{1}{4}, \frac{5}{8}]$ | $[6]$ |
| 7 | $[Y, X, -Z]$ | $[\frac{1}{2}, \frac{3}{4}, \frac{3}{8}]$ | $[7]$ |
| 8 | $[-Y, -X, -Z]$ | $[\frac{1}{2}, \frac{3}{4}, \frac{3}{8}]$ | $[8]$ |
| 9 | $[-X, -Y, -Z]$ | $[0, \frac{3}{4}, \frac{5}{8}]$ | $[9]$ |
| 10 | $[X, Y, -Z]$ | $[0, \frac{3}{4}, \frac{5}{8}]$ | $[10]$ |
| 11 | $[Y, -X, -Z]$ | $[0, \frac{1}{4}, \frac{3}{8}]$ | $[11]$ |
| 12 | $[-Y, X, -Z]$ | $[0, \frac{1}{4}, \frac{3}{8}]$ | $[12]$ |
| 13 | $[X, -Y, Z]$ | $[\frac{1}{2}, \frac{3}{4}, \frac{3}{8}]$ | $[13]$ |
| 14 | $[-X, Y, Z]$ | $[\frac{1}{2}, \frac{3}{4}, \frac{3}{8}]$ | $[14]$ |
| 15 | $[-Y, -X, Z]$ | $[\frac{1}{2}, \frac{1}{4}, \frac{5}{8}]$ | $[15]$ |
| 16 | $[Y, X, Z]$ | $[\frac{1}{2}, \frac{1}{4}, \frac{5}{8}]$ | $[16]$ |

Table 4: Wyckoff bond: 8a@8b

| No. | vector | center | mapping |
|-----|---------------|---------------------------------|----------------------|
| 1 | $[X, X, 0]$ | $[0, \frac{1}{4}, \frac{1}{8}]$ | $[1, -2, 7, -8]$ |
| 2 | $[-X, X, 0]$ | $[0, \frac{3}{4}, \frac{3}{8}]$ | $[3, -4, 5, -6]$ |
| 3 | $[-X, -X, 0]$ | $[0, \frac{3}{4}, \frac{7}{8}]$ | $[9, -10, 15, -16]$ |
| 4 | $[X, -X, 0]$ | $[0, \frac{1}{4}, \frac{5}{8}]$ | $[11, -12, 13, -14]$ |

Table 5: Wyckoff bond: 8b@8b

| No. | vector | center | mapping |
|-----|---------------|---------------------------------|----------------------|
| 1 | $[X, -X, 0]$ | $[0, \frac{1}{4}, \frac{1}{8}]$ | $[1, -2, -7, 8]$ |
| 2 | $[X, X, 0]$ | $[0, \frac{3}{4}, \frac{3}{8}]$ | $[3, -4, -5, 6]$ |
| 3 | $[-X, X, 0]$ | $[0, \frac{3}{4}, \frac{7}{8}]$ | $[9, -10, -15, 16]$ |
| 4 | $[-X, -X, 0]$ | $[0, \frac{1}{4}, \frac{5}{8}]$ | $[11, -12, -13, 14]$ |

Table 6: Wyckoff bond: 8c@8b

| No. | vector | center | mapping |
|-----|--------------|---------------------------------|----------------------|
| 1 | $[0, 0, Z]$ | $[0, \frac{1}{4}, \frac{1}{8}]$ | $[1, 2, -7, -8]$ |
| 2 | $[0, 0, Z]$ | $[0, \frac{3}{4}, \frac{3}{8}]$ | $[3, 4, -5, -6]$ |
| 3 | $[0, 0, -Z]$ | $[0, \frac{3}{4}, \frac{7}{8}]$ | $[9, 10, -15, -16]$ |
| 4 | $[0, 0, -Z]$ | $[0, \frac{1}{4}, \frac{5}{8}]$ | $[11, 12, -13, -14]$ |

Table 7: Wyckoff bond: 16d@8b

| No. | vector | center | mapping |
|-----|----------------|---------------------------------|-------------|
| 1 | $[X, X, Z]$ | $[0, \frac{1}{4}, \frac{1}{8}]$ | $[1, -8]$ |
| 2 | $[-X, -X, Z]$ | $[0, \frac{1}{4}, \frac{1}{8}]$ | $[2, -7]$ |
| 3 | $[-X, X, Z]$ | $[0, \frac{3}{4}, \frac{3}{8}]$ | $[3, -6]$ |
| 4 | $[X, -X, Z]$ | $[0, \frac{3}{4}, \frac{3}{8}]$ | $[4, -5]$ |
| 5 | $[-X, -X, -Z]$ | $[0, \frac{3}{4}, \frac{7}{8}]$ | $[9, -16]$ |
| 6 | $[X, X, -Z]$ | $[0, \frac{3}{4}, \frac{7}{8}]$ | $[10, -15]$ |
| 7 | $[X, -X, -Z]$ | $[0, \frac{1}{4}, \frac{5}{8}]$ | $[11, -14]$ |
| 8 | $[-X, X, -Z]$ | $[0, \frac{1}{4}, \frac{5}{8}]$ | $[12, -13]$ |

Table 8: Wyckoff bond: **16e@8b**

| No. | vector | center | mapping |
|-----|----------------|---------------------------------|-------------|
| 1 | $[X, -X, Z]$ | $[0, \frac{1}{4}, \frac{1}{8}]$ | $[1, -7]$ |
| 2 | $[-X, X, Z]$ | $[0, \frac{1}{4}, \frac{1}{8}]$ | $[2, -8]$ |
| 3 | $[X, X, Z]$ | $[0, \frac{3}{4}, \frac{3}{8}]$ | $[3, -5]$ |
| 4 | $[-X, -X, Z]$ | $[0, \frac{3}{4}, \frac{3}{8}]$ | $[4, -6]$ |
| 5 | $[-X, X, -Z]$ | $[0, \frac{3}{4}, \frac{7}{8}]$ | $[9, -15]$ |
| 6 | $[X, -X, -Z]$ | $[0, \frac{3}{4}, \frac{7}{8}]$ | $[10, -16]$ |
| 7 | $[-X, -X, -Z]$ | $[0, \frac{1}{4}, \frac{5}{8}]$ | $[11, -13]$ |
| 8 | $[X, X, -Z]$ | $[0, \frac{1}{4}, \frac{5}{8}]$ | $[12, -14]$ |

Table 9: Wyckoff bond: **16f@8b**

| No. | vector | center | mapping |
|-----|---------------|---------------------------------|-------------|
| 1 | $[X, Y, 0]$ | $[0, \frac{1}{4}, \frac{1}{8}]$ | $[1, -2]$ |
| 2 | $[-Y, X, 0]$ | $[0, \frac{3}{4}, \frac{3}{8}]$ | $[3, -4]$ |
| 3 | $[-X, Y, 0]$ | $[0, \frac{3}{4}, \frac{3}{8}]$ | $[5, -6]$ |
| 4 | $[Y, X, 0]$ | $[0, \frac{1}{4}, \frac{1}{8}]$ | $[7, -8]$ |
| 5 | $[-X, -Y, 0]$ | $[0, \frac{3}{4}, \frac{7}{8}]$ | $[9, -10]$ |
| 6 | $[Y, -X, 0]$ | $[0, \frac{1}{4}, \frac{5}{8}]$ | $[11, -12]$ |
| 7 | $[X, -Y, 0]$ | $[0, \frac{1}{4}, \frac{5}{8}]$ | $[13, -14]$ |
| 8 | $[-Y, -X, 0]$ | $[0, \frac{3}{4}, \frac{7}{8}]$ | $[15, -16]$ |

Table 10: Wyckoff bond: **32g@8b**

| No. | vector | center | mapping |
|-----|----------------|---------------------------------|---------|
| 1 | $[X, Y, Z]$ | $[0, \frac{1}{4}, \frac{1}{8}]$ | $[1]$ |
| 2 | $[-X, -Y, Z]$ | $[0, \frac{1}{4}, \frac{1}{8}]$ | $[2]$ |
| 3 | $[-Y, X, Z]$ | $[0, \frac{3}{4}, \frac{3}{8}]$ | $[3]$ |
| 4 | $[Y, -X, Z]$ | $[0, \frac{3}{4}, \frac{3}{8}]$ | $[4]$ |
| 5 | $[-X, Y, -Z]$ | $[0, \frac{3}{4}, \frac{3}{8}]$ | $[5]$ |
| 6 | $[X, -Y, -Z]$ | $[0, \frac{3}{4}, \frac{3}{8}]$ | $[6]$ |
| 7 | $[Y, X, -Z]$ | $[0, \frac{1}{4}, \frac{1}{8}]$ | $[7]$ |
| 8 | $[-Y, -X, -Z]$ | $[0, \frac{1}{4}, \frac{1}{8}]$ | $[8]$ |
| 9 | $[-X, -Y, -Z]$ | $[0, \frac{3}{4}, \frac{7}{8}]$ | $[9]$ |
| 10 | $[X, Y, -Z]$ | $[0, \frac{3}{4}, \frac{7}{8}]$ | $[10]$ |
| 11 | $[Y, -X, -Z]$ | $[0, \frac{1}{4}, \frac{5}{8}]$ | $[11]$ |
| 12 | $[-Y, X, -Z]$ | $[0, \frac{1}{4}, \frac{5}{8}]$ | $[12]$ |
| 13 | $[X, -Y, Z]$ | $[0, \frac{1}{4}, \frac{5}{8}]$ | $[13]$ |
| 14 | $[-X, Y, Z]$ | $[0, \frac{1}{4}, \frac{5}{8}]$ | $[14]$ |
| 15 | $[-Y, -X, Z]$ | $[0, \frac{3}{4}, \frac{7}{8}]$ | $[15]$ |
| 16 | $[Y, X, Z]$ | $[0, \frac{3}{4}, \frac{7}{8}]$ | $[16]$ |

* Wyckoff site: 16c, site symmetry: -1

Table 11: Wyckoff bond: 16a@16c

| No. | vector | center | mapping |
|-----|----------------|---|------------|
| 1 | $[X, Y, Z]$ | $[0, 0, 0]$ | $[1, -9]$ |
| 2 | $[-X, -Y, Z]$ | $[\frac{1}{2}, 0, \frac{1}{2}]$ | $[2, -10]$ |
| 3 | $[-Y, X, Z]$ | $[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$ | $[3, -11]$ |
| 4 | $[Y, -X, Z]$ | $[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}]$ | $[4, -12]$ |
| 5 | $[-X, Y, -Z]$ | $[\frac{1}{2}, 0, 0]$ | $[5, -13]$ |
| 6 | $[X, -Y, -Z]$ | $[0, 0, \frac{1}{2}]$ | $[6, -14]$ |
| 7 | $[Y, X, -Z]$ | $[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$ | $[7, -15]$ |
| 8 | $[-Y, -X, -Z]$ | $[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$ | $[8, -16]$ |

* Wyckoff site: 16d, site symmetry: $2..$

Table 12: Wyckoff bond: 16a@16d

| No. | vector | center | mapping |
|-----|---------------|---|-------------|
| 1 | $[X, Y, 0]$ | $[0, \frac{1}{4}, z]$ | $[1, -2]$ |
| 2 | $[-Y, X, 0]$ | $[0, \frac{3}{4}, z + \frac{1}{4}]$ | $[3, -4]$ |
| 3 | $[-X, Y, 0]$ | $[\frac{1}{2}, \frac{1}{4}, -z]$ | $[5, -6]$ |
| 4 | $[Y, X, 0]$ | $[\frac{1}{2}, \frac{3}{4}, \frac{3}{4} - z]$ | $[7, -8]$ |
| 5 | $[-X, -Y, 0]$ | $[0, \frac{3}{4}, -z]$ | $[9, -10]$ |
| 6 | $[Y, -X, 0]$ | $[0, \frac{1}{4}, \frac{3}{4} - z]$ | $[11, -12]$ |
| 7 | $[X, -Y, 0]$ | $[\frac{1}{2}, \frac{3}{4}, z]$ | $[13, -14]$ |
| 8 | $[-Y, -X, 0]$ | $[\frac{1}{2}, \frac{1}{4}, z + \frac{1}{4}]$ | $[15, -16]$ |

Table 13: Wyckoff bond: 16b@16d

| No. | vector | center | mapping |
|-----|--------------|---|------------|
| 1 | $[0, 0, Z]$ | $[0, \frac{1}{4}, z]$ | $[1, 2]$ |
| 2 | $[0, 0, Z]$ | $[0, \frac{3}{4}, z + \frac{1}{4}]$ | $[3, 4]$ |
| 3 | $[0, 0, -Z]$ | $[\frac{1}{2}, \frac{1}{4}, -z]$ | $[5, 6]$ |
| 4 | $[0, 0, -Z]$ | $[\frac{1}{2}, \frac{3}{4}, \frac{3}{4} - z]$ | $[7, 8]$ |
| 5 | $[0, 0, -Z]$ | $[0, \frac{3}{4}, -z]$ | $[9, 10]$ |
| 6 | $[0, 0, -Z]$ | $[0, \frac{1}{4}, \frac{3}{4} - z]$ | $[11, 12]$ |
| 7 | $[0, 0, Z]$ | $[\frac{1}{2}, \frac{3}{4}, z]$ | $[13, 14]$ |
| 8 | $[0, 0, Z]$ | $[\frac{1}{2}, \frac{1}{4}, z + \frac{1}{4}]$ | $[15, 16]$ |

Table 14: Wyckoff bond: 32c@16d

| 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 | $[-Y, X, Z]$ | $[0, \frac{3}{4}, z + \frac{1}{4}]$ | [3] |
| 4 | $[Y, -X, Z]$ | $[0, \frac{3}{4}, z + \frac{1}{4}]$ | [4] |
| 5 | $[-X, Y, -Z]$ | $[\frac{1}{2}, \frac{1}{4}, -z]$ | [5] |
| 6 | $[X, -Y, -Z]$ | $[\frac{1}{2}, \frac{1}{4}, -z]$ | [6] |
| 7 | $[Y, X, -Z]$ | $[\frac{1}{2}, \frac{3}{4}, \frac{3}{4} - z]$ | [7] |
| 8 | $[-Y, -X, -Z]$ | $[\frac{1}{2}, \frac{3}{4}, \frac{3}{4} - z]$ | [8] |
| 9 | $[-X, -Y, -Z]$ | $[0, \frac{3}{4}, -z]$ | [9] |
| 10 | $[X, Y, -Z]$ | $[0, \frac{3}{4}, -z]$ | [10] |
| 11 | $[Y, -X, -Z]$ | $[0, \frac{1}{4}, \frac{3}{4} - z]$ | [11] |
| 12 | $[-Y, X, -Z]$ | $[0, \frac{1}{4}, \frac{3}{4} - z]$ | [12] |
| 13 | $[X, -Y, Z]$ | $[\frac{1}{2}, \frac{3}{4}, z]$ | [13] |
| 14 | $[-X, Y, Z]$ | $[\frac{1}{2}, \frac{3}{4}, z]$ | [14] |
| 15 | $[-Y, -X, Z]$ | $[\frac{1}{2}, \frac{1}{4}, z + \frac{1}{4}]$ | [15] |
| 16 | $[Y, X, Z]$ | $[\frac{1}{2}, \frac{1}{4}, z + \frac{1}{4}]$ | [16] |

* Wyckoff site: 16e, site symmetry: .2.

Table 15: Wyckoff bond: 16a@16e

| No. | vector | center | mapping |
|-----|---------------|---|-----------|
| 1 | $[0, X, Z]$ | $[x, 0, \frac{1}{4}]$ | [1, -6] |
| 2 | $[0, -X, Z]$ | $[\frac{1}{2} - x, 0, \frac{3}{4}]$ | [2, -5] |
| 3 | $[-X, 0, Z]$ | $[\frac{1}{4}, x + \frac{3}{4}, \frac{1}{2}]$ | [3, -7] |
| 4 | $[X, 0, Z]$ | $[\frac{1}{4}, \frac{1}{4} - x, 0]$ | [4, -8] |
| 5 | $[0, -X, -Z]$ | $[-x, 0, \frac{3}{4}]$ | [9, -14] |
| 6 | $[0, X, -Z]$ | $[x + \frac{1}{2}, 0, \frac{1}{4}]$ | [10, -13] |
| 7 | $[X, 0, -Z]$ | $[\frac{3}{4}, \frac{1}{4} - x, \frac{1}{2}]$ | [11, -15] |
| 8 | $[-X, 0, -Z]$ | $[\frac{3}{4}, x + \frac{3}{4}, 0]$ | [12, -16] |

Table 16: Wyckoff bond: 16b@16e

| No. | vector | center | mapping |
|-----|--------------|---|----------|
| 1 | $[X, 0, 0]$ | $[x, 0, \frac{1}{4}]$ | [1, 6] |
| 2 | $[-X, 0, 0]$ | $[\frac{1}{2} - x, 0, \frac{3}{4}]$ | [2, 5] |
| 3 | $[0, X, 0]$ | $[\frac{1}{4}, x + \frac{3}{4}, \frac{1}{2}]$ | [3, 7] |
| 4 | $[0, -X, 0]$ | $[\frac{1}{4}, \frac{1}{4} - x, 0]$ | [4, 8] |
| 5 | $[-X, 0, 0]$ | $[-x, 0, \frac{3}{4}]$ | [9, 14] |
| 6 | $[X, 0, 0]$ | $[x + \frac{1}{2}, 0, \frac{1}{4}]$ | [10, 13] |
| 7 | $[0, -X, 0]$ | $[\frac{3}{4}, \frac{1}{4} - x, \frac{1}{2}]$ | [11, 15] |
| 8 | $[0, X, 0]$ | $[\frac{3}{4}, x + \frac{3}{4}, 0]$ | [12, 16] |

Table 17: Wyckoff bond: **32c@16e**

| No. | vector | center | mapping |
|-----|----------------|---|---------|
| 1 | $[X, Y, Z]$ | $[x, 0, \frac{1}{4}]$ | [1] |
| 2 | $[-X, -Y, Z]$ | $[\frac{1}{2} - x, 0, \frac{3}{4}]$ | [2] |
| 3 | $[-Y, X, Z]$ | $[\frac{1}{4}, x + \frac{3}{4}, \frac{1}{2}]$ | [3] |
| 4 | $[Y, -X, Z]$ | $[\frac{1}{4}, \frac{1}{4} - x, 0]$ | [4] |
| 5 | $[-X, Y, -Z]$ | $[\frac{1}{2} - x, 0, \frac{3}{4}]$ | [5] |
| 6 | $[X, -Y, -Z]$ | $[x, 0, \frac{1}{4}]$ | [6] |
| 7 | $[Y, X, -Z]$ | $[\frac{1}{4}, x + \frac{3}{4}, \frac{1}{2}]$ | [7] |
| 8 | $[-Y, -X, -Z]$ | $[\frac{1}{4}, \frac{1}{4} - x, 0]$ | [8] |
| 9 | $[-X, -Y, -Z]$ | $[-x, 0, \frac{3}{4}]$ | [9] |
| 10 | $[X, Y, -Z]$ | $[x + \frac{1}{2}, 0, \frac{1}{4}]$ | [10] |
| 11 | $[Y, -X, -Z]$ | $[\frac{3}{4}, \frac{1}{4} - x, \frac{1}{2}]$ | [11] |
| 12 | $[-Y, X, -Z]$ | $[\frac{3}{4}, x + \frac{3}{4}, 0]$ | [12] |
| 13 | $[X, -Y, Z]$ | $[x + \frac{1}{2}, 0, \frac{1}{4}]$ | [13] |
| 14 | $[-X, Y, Z]$ | $[-x, 0, \frac{3}{4}]$ | [14] |
| 15 | $[-Y, -X, Z]$ | $[\frac{3}{4}, \frac{1}{4} - x, \frac{1}{2}]$ | [15] |
| 16 | $[Y, X, Z]$ | $[\frac{3}{4}, x + \frac{3}{4}, 0]$ | [16] |

* Wyckoff site: **16f**, site symmetry: $\dots 2$

Table 18: Wyckoff bond: **16a@16f**

| No. | vector | center | mapping |
|-----|----------------|---|-----------|
| 1 | $[X, -X, Z]$ | $[x, x + \frac{1}{4}, \frac{1}{8}]$ | [1, -7] |
| 2 | $[-X, X, Z]$ | $[\frac{1}{2} - x, \frac{3}{4} - x, \frac{5}{8}]$ | [2, -8] |
| 3 | $[X, X, Z]$ | $[-x, x + \frac{3}{4}, \frac{3}{8}]$ | [3, -5] |
| 4 | $[-X, -X, Z]$ | $[x + \frac{1}{2}, \frac{1}{4} - x, \frac{7}{8}]$ | [4, -6] |
| 5 | $[-X, X, -Z]$ | $[-x, \frac{3}{4} - x, \frac{7}{8}]$ | [9, -15] |
| 6 | $[X, -X, -Z]$ | $[x + \frac{1}{2}, x + \frac{1}{4}, \frac{3}{8}]$ | [10, -16] |
| 7 | $[-X, -X, -Z]$ | $[x, \frac{1}{4} - x, \frac{5}{8}]$ | [11, -13] |
| 8 | $[X, X, -Z]$ | $[\frac{1}{2} - x, x + \frac{3}{4}, \frac{1}{8}]$ | [12, -14] |

Table 19: Wyckoff bond: **16b@16f**

| No. | vector | center | mapping |
|-----|---------------|---|----------|
| 1 | $[X, X, 0]$ | $[x, x + \frac{1}{4}, \frac{1}{8}]$ | [1, 7] |
| 2 | $[-X, -X, 0]$ | $[\frac{1}{2} - x, \frac{3}{4} - x, \frac{5}{8}]$ | [2, 8] |
| 3 | $[-X, X, 0]$ | $[-x, x + \frac{3}{4}, \frac{3}{8}]$ | [3, 5] |
| 4 | $[X, -X, 0]$ | $[x + \frac{1}{2}, \frac{1}{4} - x, \frac{7}{8}]$ | [4, 6] |
| 5 | $[-X, -X, 0]$ | $[-x, \frac{3}{4} - x, \frac{7}{8}]$ | [9, 15] |
| 6 | $[X, X, 0]$ | $[x + \frac{1}{2}, x + \frac{1}{4}, \frac{3}{8}]$ | [10, 16] |

continued ...

Table 19

| No. | vector | center | mapping |
|-----|--------------|---|----------|
| 7 | $[X, -X, 0]$ | $[x, \frac{1}{4} - x, \frac{5}{8}]$ | [11, 13] |
| 8 | $[-X, X, 0]$ | $[\frac{1}{2} - x, x + \frac{3}{4}, \frac{1}{8}]$ | [12, 14] |

Table 20: Wyckoff bond: 32c@16f

| No. | vector | center | mapping |
|-----|----------------|---|---------|
| 1 | $[X, Y, Z]$ | $[x, x + \frac{1}{4}, \frac{1}{8}]$ | [1] |
| 2 | $[-X, -Y, Z]$ | $[\frac{1}{2} - x, \frac{3}{4} - x, \frac{5}{8}]$ | [2] |
| 3 | $[-Y, X, Z]$ | $[-x, x + \frac{3}{4}, \frac{3}{8}]$ | [3] |
| 4 | $[Y, -X, Z]$ | $[x + \frac{1}{2}, \frac{1}{4} - x, \frac{7}{8}]$ | [4] |
| 5 | $[-X, Y, -Z]$ | $[-x, x + \frac{3}{4}, \frac{3}{8}]$ | [5] |
| 6 | $[X, -Y, -Z]$ | $[x + \frac{1}{2}, \frac{1}{4} - x, \frac{7}{8}]$ | [6] |
| 7 | $[Y, X, -Z]$ | $[x, x + \frac{1}{4}, \frac{1}{8}]$ | [7] |
| 8 | $[-Y, -X, -Z]$ | $[\frac{1}{2} - x, \frac{3}{4} - x, \frac{5}{8}]$ | [8] |
| 9 | $[-X, -Y, -Z]$ | $[-x, \frac{3}{4} - x, \frac{7}{8}]$ | [9] |
| 10 | $[X, Y, -Z]$ | $[x + \frac{1}{2}, x + \frac{1}{4}, \frac{3}{8}]$ | [10] |
| 11 | $[Y, -X, -Z]$ | $[x, \frac{1}{4} - x, \frac{5}{8}]$ | [11] |
| 12 | $[-Y, X, -Z]$ | $[\frac{1}{2} - x, x + \frac{3}{4}, \frac{1}{8}]$ | [12] |
| 13 | $[X, -Y, Z]$ | $[x, \frac{1}{4} - x, \frac{5}{8}]$ | [13] |
| 14 | $[-X, Y, Z]$ | $[\frac{1}{2} - x, x + \frac{3}{4}, \frac{1}{8}]$ | [14] |
| 15 | $[-Y, -X, Z]$ | $[-x, \frac{3}{4} - x, \frac{7}{8}]$ | [15] |
| 16 | $[Y, X, Z]$ | $[x + \frac{1}{2}, x + \frac{1}{4}, \frac{3}{8}]$ | [16] |

* Wyckoff site: 32g, site symmetry: 1

Table 21: Wyckoff bond: 32a@32g

| No. | vector | center | mapping |
|-----|----------------|---|---------|
| 1 | $[X, Y, Z]$ | $[x, y, z]$ | [1] |
| 2 | $[-X, -Y, Z]$ | $[\frac{1}{2} - x, -y, z + \frac{1}{2}]$ | [2] |
| 3 | $[-Y, X, Z]$ | $[\frac{1}{4} - y, x + \frac{3}{4}, z + \frac{1}{4}]$ | [3] |
| 4 | $[Y, -X, Z]$ | $[y + \frac{1}{4}, \frac{1}{4} - x, z + \frac{3}{4}]$ | [4] |
| 5 | $[-X, Y, -Z]$ | $[\frac{1}{2} - x, y, -z]$ | [5] |
| 6 | $[X, -Y, -Z]$ | $[x, -y, \frac{1}{2} - z]$ | [6] |
| 7 | $[Y, X, -Z]$ | $[y + \frac{1}{4}, x + \frac{3}{4}, \frac{3}{4} - z]$ | [7] |
| 8 | $[-Y, -X, -Z]$ | $[\frac{1}{4} - y, \frac{1}{4} - x, \frac{1}{4} - z]$ | [8] |
| 9 | $[-X, -Y, -Z]$ | $[-x, -y, -z]$ | [9] |
| 10 | $[X, Y, -Z]$ | $[x + \frac{1}{2}, y, \frac{1}{2} - z]$ | [10] |
| 11 | $[Y, -X, -Z]$ | $[y + \frac{3}{4}, \frac{1}{4} - x, \frac{3}{4} - z]$ | [11] |
| 12 | $[-Y, X, -Z]$ | $[\frac{3}{4} - y, x + \frac{3}{4}, \frac{1}{4} - z]$ | [12] |
| 13 | $[X, -Y, Z]$ | $[x + \frac{1}{2}, -y, z]$ | [13] |
| 14 | $[-X, Y, Z]$ | $[-x, y, z + \frac{1}{2}]$ | [14] |

continued ...

Table 21

| No. | vector | center | mapping |
|-----|---------------|---|---------|
| 15 | $[-Y, -X, Z]$ | $[\frac{3}{4} - y, \frac{1}{4} - x, z + \frac{1}{4}]$ | [15] |
| 16 | $[Y, X, Z]$ | $[y + \frac{3}{4}, x + \frac{3}{4}, z + \frac{3}{4}]$ | [16] |