

SG No. 138 D_{4h}^{16} $P4_2/nmc$ [tetragonal]

* plus set: +[0, 0, 0]

* Wyckoff site: 4a, site symmetry: 2.22

Table 1: Wyckoff bond: 4a@4a

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

Table 2: Wyckoff bond: 4b@4a

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

Table 3: Wyckoff bond: 4c@4a

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

Table 4: Wyckoff bond: 8d@4a

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

Table 5: Wyckoff bond: 8e@4a

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

Table 6: Wyckoff bond: 8f@4a

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

Table 7: Wyckoff bond: 16g@4a

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

* Wyckoff site: **4b**, site symmetry: **-4..**

Table 8: Wyckoff bond: **4a@4b**

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

Table 9: Wyckoff bond: **8b@4b**

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

Table 10: Wyckoff bond: **16c@4b**

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

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

Table 11: Wyckoff bond: 4a@4c

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

Table 12: Wyckoff bond: 4b@4c

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

Table 13: Wyckoff bond: 8c@4c

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

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

Table 14: Wyckoff bond: 4a@4d

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

Table 15: Wyckoff bond: 4b@4d

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

Table 16: Wyckoff bond: 8c@4d

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

* Wyckoff site: 4e, site symmetry: 2..mm

Table 17: Wyckoff bond: 4a@4e

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

Table 18: Wyckoff bond: 4b@4e

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

Table 19: Wyckoff bond: 8c@4e

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

Table 20: Wyckoff bond: 8d@4e

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

Table 21: Wyckoff bond: 16e@4e

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

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

Table 22: Wyckoff bond: 8a@8f

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

Table 23: Wyckoff bond: 8b@8f

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

Table 24: Wyckoff bond: 16c@8f

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

continued ...

Table 24

No.	vector	center	mapping
16	[Y, X, Z]	[$\frac{1}{4}, \frac{3}{4}, z$]	[16]

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

Table 25: Wyckoff bond: 8a@8g

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

Table 26: Wyckoff bond: 8b@8g

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

Table 27: Wyckoff bond: 16c@8g

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

continued ...

Table 27

No.	vector	center	mapping
10	$[X, Y, -Z]$	$[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]$	[10]
11	$[Y, -X, -Z]$	$[\frac{1}{2} - x, -x, 0]$	[11]
12	$[-Y, X, -Z]$	$[x, x + \frac{1}{2}, 0]$	[12]
13	$[X, -Y, Z]$	$[x, x + \frac{1}{2}, 0]$	[13]
14	$[-X, Y, Z]$	$[\frac{1}{2} - x, -x, 0]$	[14]
15	$[-Y, -X, Z]$	$[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]$	[15]
16	$[Y, X, Z]$	$[-x, x, \frac{1}{2}]$	[16]

* Wyckoff site: 8h, site symmetry: ...2

Table 28: Wyckoff bond: 8a@8h

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

Table 29: Wyckoff bond: 8b@8h

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

Table 30: Wyckoff bond: 16c@8h

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, -x, 0]$	[1]
2	$[-X, -Y, Z]$	$[\frac{1}{2} - x, x + \frac{1}{2}, 0]$	[2]
3	$[-Y, X, Z]$	$[x + \frac{1}{2}, x, \frac{1}{2}]$	[3]

continued ...

Table 30

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

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

Table 31: Wyckoff bond: 8a@8i

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

Table 32: Wyckoff bond: 8b@8i

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

Table 33: Wyckoff bond: 16c@8i

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

* Wyckoff site: 16j, site symmetry: 1

Table 34: Wyckoff bond: 16a@16j

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