

PG No. 11 C_{4h} 4/ m [tetragonal]

* Wyckoff site: 2a, site symmetry: 4..

Table 1: Wyckoff bond: 2a@2a

No.	vector	center	mapping
1	[0, 0, Z]	[0, 0, z]	[1, 2, 3, 4]
2	[0, 0, $-Z$]	[0, 0, $-z$]	[5, 6, 7, 8]

Table 2: Wyckoff bond: 4b@2a

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

Table 3: Wyckoff bond: 8c@2a

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

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

Table 4: Wyckoff bond: 4a@4b

No.	vector	center	mapping
1	[X , Y , 0]	[x , y , 0]	[1, 6]
2	[$-X$, $-Y$, 0]	[$-x$, $-y$, 0]	[2, 5]
3	[$-Y$, X , 0]	[$-y$, x , 0]	[3, 8]
4	[Y , $-X$, 0]	[y , $-x$, 0]	[4, 7]

Table 5: Wyckoff bond: 4b@4b

No.	vector	center	mapping
1	[0, 0, Z]	[x, y, 0]	[1, -6]
2	[0, 0, Z]	[-x, -y, 0]	[2, -5]
3	[0, 0, Z]	[-y, x, 0]	[3, -8]
4	[0, 0, Z]	[y, -x, 0]	[4, -7]

Table 6: Wyckoff bond: 8c@4b

No.	vector	center	mapping
1	[X, Y, Z]	[x, y, 0]	[1]
2	[-X, -Y, Z]	[-x, -y, 0]	[2]
3	[-Y, X, Z]	[-y, x, 0]	[3]
4	[Y, -X, Z]	[y, -x, 0]	[4]
5	[-X, -Y, -Z]	[-x, -y, 0]	[5]
6	[X, Y, -Z]	[x, y, 0]	[6]
7	[Y, -X, -Z]	[y, -x, 0]	[7]
8	[-Y, X, -Z]	[-y, x, 0]	[8]

* Wyckoff site: 8c, site symmetry: 1

Table 7: Wyckoff bond: 8a@8c

No.	vector	center	mapping
1	[X, Y, Z]	[x, y, z]	[1]
2	[-X, -Y, Z]	[-x, -y, z]	[2]
3	[-Y, X, Z]	[-y, x, z]	[3]
4	[Y, -X, Z]	[y, -x, z]	[4]
5	[-X, -Y, -Z]	[-x, -y, -z]	[5]
6	[X, Y, -Z]	[x, y, -z]	[6]
7	[Y, -X, -Z]	[y, -x, -z]	[7]
8	[-Y, X, -Z]	[-y, x, -z]	[8]