

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	$[-Y, X, -Z]$	$[-y, x, -z]$	$[8]$