

SG No. 110  $C_{4v}^{12}$   $I4_1cd$  [ tetragonal ]

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

\* Wyckoff site: **8a**, site symmetry:  $2..$

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

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

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

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

Table 3: Wyckoff bond: **16c@8a**

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

\* Wyckoff site: **16b**, site symmetry:  $1$

Table 4: Wyckoff bond: **16a@16b**

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

*continued ...*

Table 4

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