

SG No. 92  $D_4^4$   $P4_12_12$  [ tetragonal ]

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

\* Wyckoff site: 4a, site symmetry:  $\dots 2$

Table 1: Wyckoff bond: 4a@4a

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

Table 2: Wyckoff bond: 4b@4a

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

Table 3: Wyckoff bond: 8c@4a

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

\* Wyckoff site: 8b, site symmetry: 1

Table 4: Wyckoff bond: 8a@8b

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

*continued ...*

Table 4

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