

SG No. 96  $D_4^8$   $P4_3212$  [ tetragonal ]

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

\* Wyckoff site: 4a, site symmetry: . . 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	[ $X, X, Z$ ]	[ $\frac{1}{2} - x, x + \frac{1}{2}, \frac{3}{4}$ ]	[3, -5]
4	[ $-X, -X, Z$ ]	[ $x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{4}$ ]	[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	[ $-X, X, 0$ ]	[ $\frac{1}{2} - x, x + \frac{1}{2}, \frac{3}{4}$ ]	[3, 5]
4	[ $X, -X, 0$ ]	[ $x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{4}$ ]	[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	[ $-Y, X, Z$ ]	[ $\frac{1}{2} - x, x + \frac{1}{2}, \frac{3}{4}$ ]	[3]
4	[ $Y, -X, Z$ ]	[ $x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{4}$ ]	[4]
5	[ $-X, Y, -Z$ ]	[ $\frac{1}{2} - x, x + \frac{1}{2}, \frac{3}{4}$ ]	[5]
6	[ $X, -Y, -Z$ ]	[ $x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{4}$ ]	[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	[ $-Y, X, Z$ ]	[ $\frac{1}{2} - y, x + \frac{1}{2}, z + \frac{3}{4}$ ]	[3]
4	[ $Y, -X, Z$ ]	[ $y + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{4}$ ]	[4]
5	[ $-X, Y, -Z$ ]	[ $\frac{1}{2} - x, y + \frac{1}{2}, \frac{3}{4} - z$ ]	[5]

*continued ...*

Table 4

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