

SG No. 96 D_4^8 $P4_32_12$ [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]	$[\frac{1}{2} - x, x + \frac{1}{2}, \frac{3}{4}]$	[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]