

PG No. 18 D_3 32 (321 setting) [trigonal]

* Wyckoff site: 2a, site symmetry: 3..

Table 1: Wyckoff bond: 2a@2a

No.	vector	center	mapping
1	[0, 0, Z]	[0, 0, z]	[1, 2, 3]
2	[0, 0, -Z]	[0, 0, -z]	[4, 5, 6]

Table 2: Wyckoff bond: 6b@2a

No.	vector	center	mapping
1	[X, Y, Z]	[0, 0, z]	[1]
2	[-Y, X - Y, Z]	[0, 0, z]	[2]
3	[-X + Y, -X, Z]	[0, 0, z]	[3]
4	[Y, X, -Z]	[0, 0, -z]	[4]
5	[X - Y, -Y, -Z]	[0, 0, -z]	[5]
6	[-X, -X + Y, -Z]	[0, 0, -z]	[6]

* Wyckoff site: 3b, site symmetry: .2.

Table 3: Wyckoff bond: 3a@3b

No.	vector	center	mapping
1	[X, 2X, Z]	[x, 0, 0]	[1, -5]
2	[-2X, -X, Z]	[0, x, 0]	[2, -4]
3	[X, -X, Z]	[-x, -x, 0]	[3, -6]

Table 4: Wyckoff bond: 3b@3b

No.	vector	center	mapping
1	[X, 0, 0]	[x, 0, 0]	[1, 5]
2	[0, X, 0]	[0, x, 0]	[2, 4]
3	[-X, -X, 0]	[-x, -x, 0]	[3, 6]

Table 5: Wyckoff bond: 6c@3b

No.	vector	center	mapping
1	[X, Y, Z]	[x, 0, 0]	[1]
2	[-Y, X - Y, Z]	[0, x, 0]	[2]

continued ...

Table 5

No.	vector	center	mapping
3	$[-X + Y, -X, Z]$	$[-x, -x, 0]$	[3]
4	$[Y, X, -Z]$	$[0, x, 0]$	[4]
5	$[X - Y, -Y, -Z]$	$[x, 0, 0]$	[5]
6	$[-X, -X + Y, -Z]$	$[-x, -x, 0]$	[6]

* Wyckoff site: 6c, site symmetry: 1

Table 6: Wyckoff bond: 6a@6c

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, y, z]$	[1]
2	$[-Y, X - Y, Z]$	$[-y, x - y, z]$	[2]
3	$[-X + Y, -X, Z]$	$[-x + y, -x, z]$	[3]
4	$[Y, X, -Z]$	$[y, x, -z]$	[4]
5	$[X - Y, -Y, -Z]$	$[x - y, -y, -z]$	[5]
6	$[-X, -X + Y, -Z]$	$[-x, -x + y, -z]$	[6]