

* 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]