

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

\* Wyckoff site: **1a**, site symmetry:  $6..$

Table 1: Wyckoff bond: **1a@1a**

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

Table 2: Wyckoff bond: **3b@1a**

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

Table 3: Wyckoff bond: **6c@1a**

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	$[-X, -Y, Z]$	$[0, 0, z]$	$[4]$
5	$[Y, -X + Y, Z]$	$[0, 0, z]$	$[5]$
6	$[X - Y, X, Z]$	$[0, 0, z]$	$[6]$

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

Table 4: Wyckoff bond: **2a@2b**

No.	vector	center	mapping
1	$[0, 0, Z]$	$[\frac{1}{3}, \frac{2}{3}, z]$	$[1, 2, 3]$
2	$[0, 0, Z]$	$[\frac{2}{3}, \frac{1}{3}, z]$	$[4, 5, 6]$

Table 5: Wyckoff bond: **6b@2b**

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

*continued ...*

Table 5

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

\* Wyckoff site: 3c, site symmetry: 2..

Table 6: Wyckoff bond: 3a@3c

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

Table 7: Wyckoff bond: 3b@3c

No.	vector	center	mapping
1	$[0, 0, Z]$	$[\frac{1}{2}, 0, z]$	[1, 4]
2	$[0, 0, Z]$	$[0, \frac{1}{2}, z]$	[2, 5]
3	$[0, 0, Z]$	$[\frac{1}{2}, \frac{1}{2}, z]$	[3, 6]

Table 8: Wyckoff bond: 6c@3c

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

\* Wyckoff site: 6d, site symmetry: 1

Table 9: Wyckoff bond: 6a@6d

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]

*continued ...*

Table 9

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