

PG No. 35 $C_{3v}(1)$ $3m$ (31m setting) [trigonal]

* Wyckoff site: **1a**, site symmetry: $3.m$

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	$[X, 0, Z]$	$[0, 0, z]$	$[1, 5]$
2	$[0, X, Z]$	$[0, 0, z]$	$[2, 4]$
3	$[-X, -X, Z]$	$[0, 0, z]$	$[3, 6]$

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

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

Table 4: Wyckoff bond: **6d@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	$[Y, X, Z]$	$[0, 0, z]$	$[4]$
5	$[X - Y, -Y, Z]$	$[0, 0, z]$	$[5]$
6	$[-X, -X + Y, Z]$	$[0, 0, z]$	$[6]$

* Wyckoff site: **3b**, site symmetry: $.m$

Table 5: Wyckoff bond: **3a@3b**

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

Table 6: Wyckoff bond: **3b@3b**

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

Table 7: Wyckoff bond: **6c@3b**

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

* Wyckoff site: **6c**, site symmetry: **1**

Table 8: 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	$[-X, -X + Y, Z]$	$[-x, -x + y, z]$	$[6]$