

PG No. 19 C_{3v} $3m$ (3m1 setting) [trigonal]

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

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

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

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

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

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

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

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

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

* 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	$[X, X - Y, Z]$	$[x, x - y, z]$	$[6]$