

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]