

SG No. 147 $C_{3i}^1 P\bar{3}$ [trigonal]

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

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

Table 1: Wyckoff bond: 1a@1a

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

Table 2: Wyckoff bond: 3b@1a

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

* Wyckoff site: 1b, site symmetry: $-3..$

Table 3: Wyckoff bond: 1a@1b

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

Table 4: Wyckoff bond: 3b@1b

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

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

Table 5: Wyckoff bond: 2a@2c

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 6: Wyckoff bond: **6b@2c**

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: **2d**, site symmetry: **3..**

Table 7: Wyckoff bond: **2a@2d**

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 8: Wyckoff bond: **6b@2d**

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]
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: **3e**, site symmetry: **-1**

Table 9: Wyckoff bond: **3a@3e**

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

* Wyckoff site: **3f**, site symmetry: **-1**

Table 10: Wyckoff bond: 3a@3f

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

* Wyckoff site: 6g, site symmetry: 1

Table 11: Wyckoff bond: 6a@6g

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