

SG No. 155 D_3^7 $R32$ [trigonal]

* plus set: $+ [0, 0, 0]$, $+ [\frac{2}{3}, \frac{1}{3}, \frac{1}{3}]$, $+ [\frac{1}{3}, \frac{2}{3}, \frac{2}{3}]$

* Wyckoff site: **3a**, site symmetry: **32**

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

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

Table 2: Wyckoff bond: **9b@3a**

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

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

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

Table 4: Wyckoff bond: **18d@3a**

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

* Wyckoff site: **3b**, site symmetry: **32**

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

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

Table 6: Wyckoff bond: **9b@3b**

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

Table 7: Wyckoff bond: **9c@3b**

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

Table 8: Wyckoff bond: **18d@3b**

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

* Wyckoff site: **6c**, site symmetry: **3**.

Table 9: Wyckoff bond: **6a@6c**

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 10: Wyckoff bond: **18b@6c**

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	$[X - Y, -Y, -Z]$	$[0, 0, -z]$	$[5]$

continued ...

Table 10

No.	vector	center	mapping
6	$[-X, -X + Y, -Z]$	$[0, 0, -z]$	[6]

* Wyckoff site: **9d**, site symmetry: .2

Table 11: Wyckoff bond: **9a@9d**

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

Table 12: Wyckoff bond: **9b@9d**

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

Table 13: Wyckoff bond: **18c@9d**

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

* Wyckoff site: **9e**, site symmetry: .2

Table 14: Wyckoff bond: **9a@9e**

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

Table 15: Wyckoff bond: **9b@9e**

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

Table 16: Wyckoff bond: **18c@9e**

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

* Wyckoff site: **18f**, site symmetry: **1**

Table 17: Wyckoff bond: **18a@18f**

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]