

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]